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=> d que l12
L3                STR
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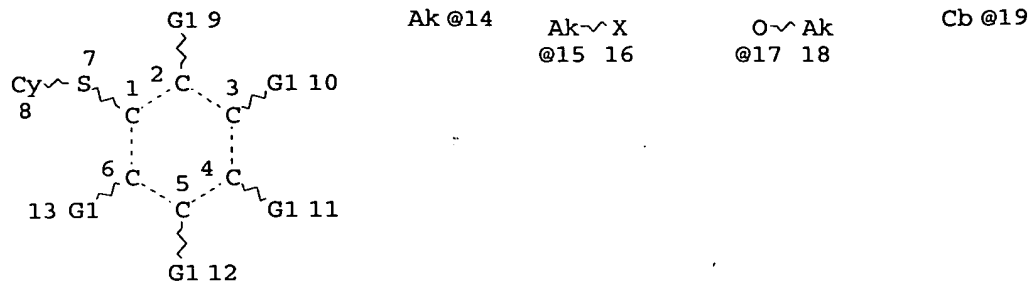

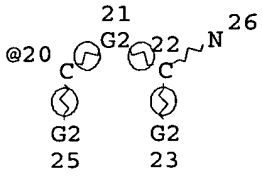


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VAR G1=H/X/14/15/17/CN/NO2/19/CHO/20
VAR G2=C/O/S/N
NODE ATTRIBUTES:
NSPEC   IS RC     AT  26
CONNECT IS E2  RC AT   7
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  18
CONNECT IS E1  RC AT  19
DEFAULT MLEVEL IS ATOM
GGCAT   IS SAT  AT  19
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  25

STEREO ATTRIBUTES: NONE
L5       1356440 SEA FILE=REGISTRY ABB=ON  PLU=ON  C6/ES AND NC5/ES
L7          6794 SEA FILE=REGISTRY SUB=L5 SSS FUL L3
L8               STR
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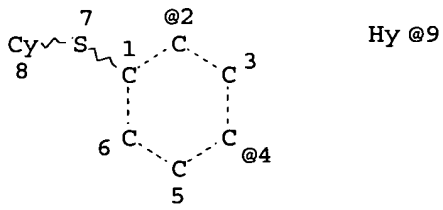


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VPA 9-2/4 U
NODE ATTRIBUTES:
CONNECT IS E2  RC AT   7
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   9
DEFAULT ECLEVEL IS LIMITED
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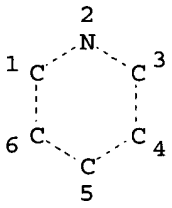
ECOUNT IS E5 C E1 N AT 9

GRAPH ATTRIBUTES:
RSPEC 6
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L9 265 SEA FILE=REGISTRY SUB=L7 SSS FUL L8
L10 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 6

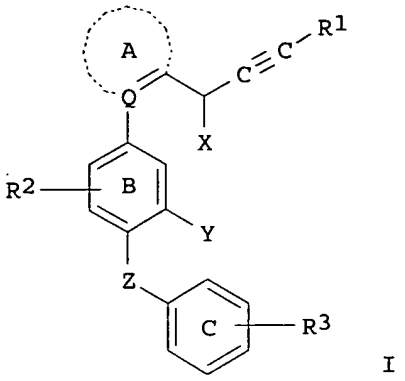
STEREO ATTRIBUTES: NONE
L11 133 SEA FILE=REGISTRY SUB=L9 SSS FUL L10
L12 19 SEA FILE=HCAPLUS ABB=ON PLU=ON L11

=> d l12 ibib abs hitstr 1-19

L12 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:72766 HCAPLUS
DOCUMENT NUMBER: 142:176543
TITLE: Preparation of arylalkyne derivatives having EDG receptor antagonist effect
INVENTOR(S): Sato, Susumu; Nakamura, Takeshi; Nara, Futoshi; Komesu, Kiyoaki
PATENT ASSIGNEE(S): Sankyo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 181 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005022986	A2	20050127	JP 2003-187530	20030630

PRIORITY APPLN. INFO.: JP 2003-187530 20030630
GI

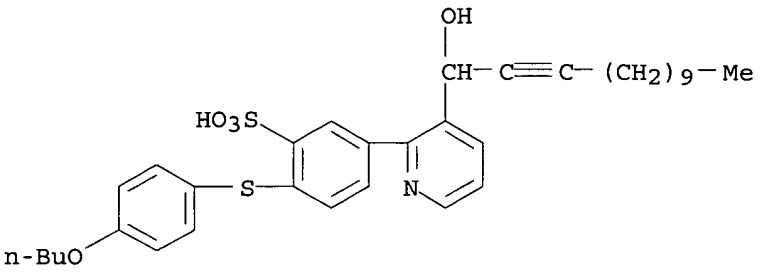


I

AB The title compds. (I), or salts or esters thereof [R1 = (un)substituted C1-17 alkyl optionally containing 1 or ≥2 of a double or triple bond, (un)substituted benzene ring, O, S, SO, SO2, and (un)substituted NH; R2 represents 1-3 substituents selected from H, HO, CO2H, NO2, halo, alkoxy, alkenyloxy, alkynyloxy, aralkyloxy, NH2, alkylamino, alkanoylamino, alkylthio, and (un)substituted C1-6 alkyl; R3 represents 1-3 substituents selected from H, HO, aralkyloxy, alkylamino, alkanoylamino, alkylthio, CO2H, NO2, halo, and (un)substituted C1-10 alkyl; X = alkylamino, HO, NH2, (un)substituted C1-6 alkoxy; Y = CO2H, SO3H, P(O)(OH)2; Z = O, S, (un)substituted NH, CO, SO, SO2, (un)substituted CH2; ring A = (un)substituted 4- to 7-membered ring containing -Q:C- as a partial structure and optionally containing 1 or ≥2 of CH:CH, N, O, (un)substituted NH, S, and CO; Q = C, N] are prepared These compds. are endothelial differentiation gene 1 (EDG-1) receptor antagonists and effective in preventing and/or treating inflammations, diseases associated with abnormal angiogenesis, cerebral vascular spasm, brain ischemia, cancer-related diseases, cerebral infarction, myocardial infarction, nephritis, pneumonia, immune diseases, Crohn's disease, colitis, or chronic diarrhea. Thus, Suzuki coupling of Me 5-bromo-2-[(4-butoxyphenyl)thio]benzoate with 2-formylphenylboronic acid in the presence of tetrakis(triphenylphosphine)palladium in a mixture of 4.6 M aqueous K2CO3 solution in 1,2-dimethoxyethane at 60° for 5 h to give 99% Me 4-[(4-butoxyphenyl)thio]-2'-formyl-1,1'-biphenyl-3-carboxylate (II). 2-[[7-(2-Propynyloxy)heptyl]oxy]tetrahydro-2H-pyran was treated with 1.6 M BuLi/hexane in THF at -78°, stirred for 10 min, treated dropwise with a solution of II in THF, and stirred for 1 h to give 78% Me 4-[(4-butoxyphenyl)thio]-2'-[1-hydroxy-4-[[7-[(tetrahydro-2H-pyran-2-yl)oxy]heptyl]oxy]-2-butynyl]-1,1'-biphenyl-3-carboxylate which was stirred in the presence of pyridinium p-toluenesulfonate in ethanol at 60° for 1 h to give 82% Me 4-[(4-butoxyphenyl)thio]-2'-[1-hydroxy-4-[(7-hydroxyheptyl)oxy]-2-butynyl]-1,1'-biphenyl-3-carboxylate (III). III was heated with NaOH in aqueous dioxane at 90° for 8 h to give 76% sodium 4-[(4-butoxyphenyl)thio]-2'-[1-hydroxy-4-[(7-hydroxyheptyl)oxy]-2-butynyl]-1,1'-biphenyl-3-carboxylate (IV). IV inhibited the sphingosine-1-phosphate-stimulated production of cAMP in CHO cells expressing Edg-1 with IC50 of 0.020 μM.

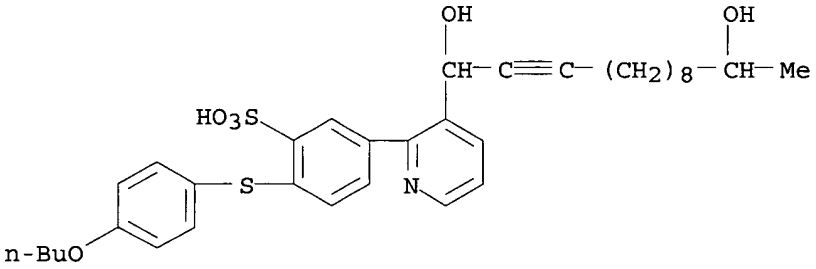
IT **832725-53-8P 832725-54-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of alkyne derivs. as EDG-1 receptor antagonists)

RN 832725-53-8 HCAPLUS
CN Benzenesulfonic acid, 2-[(4-butoxyphenyl)thio]-5-[3-(1-hydroxy-2-tridecynyl)-2-pyridinyl]-, monosodium salt (9CI) (CA INDEX NAME)



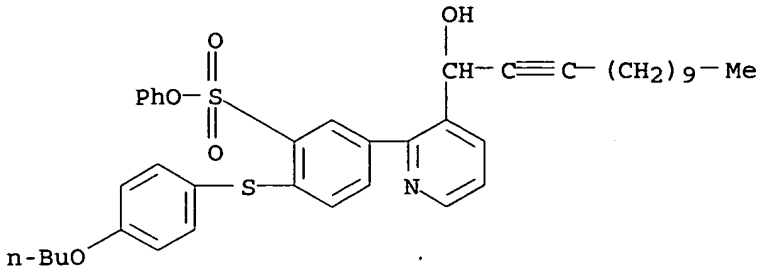
● Na

RN 832725-54-9 HCAPLUS
CN Benzenesulfonic acid, 2-[(4-butoxyphenyl)thio]-5-[3-(1,12-dihydroxy-2-tridecynyl)-2-pyridinyl]-, monosodium salt (9CI) (CA INDEX NAME)

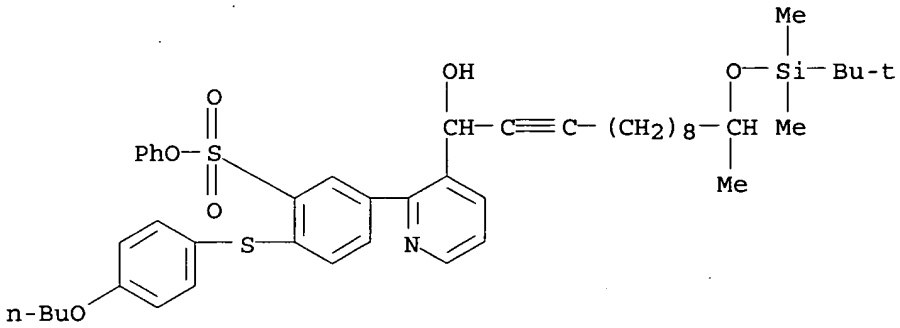


● Na

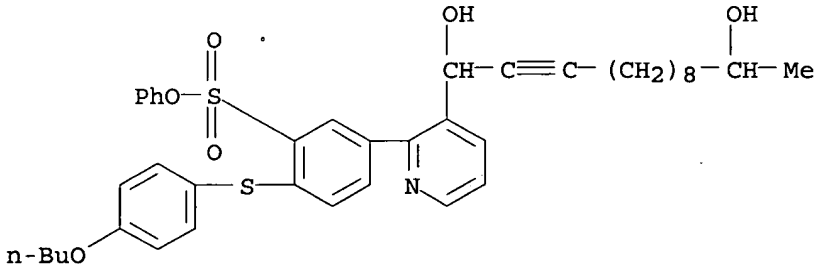
IT **832726-79-1P 832726-80-4P 832726-81-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of alkyne derivs. as EDG-1 receptor antagonists)
RN 832726-79-1 HCAPLUS
CN Benzenesulfonic acid, 2-[(4-butoxyphenyl)thio]-5-[3-(1-hydroxy-2-tridecynyl)-2-pyridinyl]-, phenyl ester (9CI) (CA INDEX NAME)



RN 832726-80-4 HCAPLUS
CN Benzenesulfonic acid, 2-[(4-butoxyphenyl)thio]-5-[3-[12-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-hydroxy-2-tridecynyl]-2-pyridinyl]-, phenyl ester (9CI) (CA INDEX NAME)

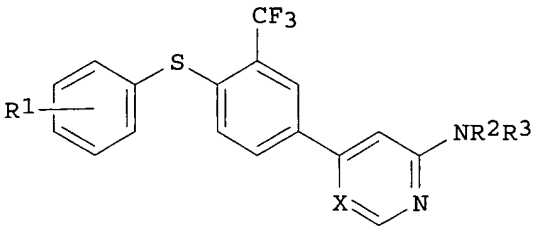


RN 832726-81-5 HCAPLUS
CN Benzenesulfonic acid, 2-[(4-butoxyphenyl)thio]-5-[3-(1,12-dihydroxy-2-tridecynyl)-2-pyridinyl]-, phenyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 2 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1068277 HCAPLUS
DOCUMENT NUMBER: 142:155913
TITLE: Amino-substituted heterocycles as isosteres of trans-cinnamides: design and synthesis of heterocyclic biaryl sulfides as potent antagonists of LFA-1/ICAM-1 binding
AUTHOR(S): Wang, Gary T.; Wang, Sheldon; Gentles, Robert; Sowin, Thomas; Leitza, Sandra; Reilly, Edward B.; von

Geldern, Thomas W.
CORPORATE SOURCE: Global Pharmaceutical Research & Development, Abbott Laboratories, Abbott Park, IL, 60064, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(1), 195-201
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:155913
GI



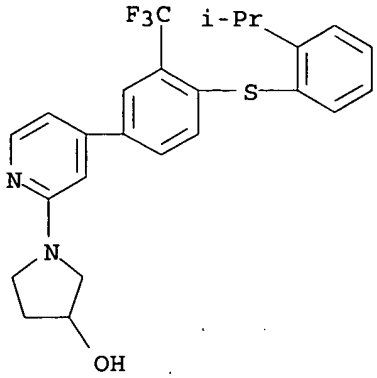
I

AB 2-Amino-4-Ph pyridine and to a lesser extent, 4-amino-6-Ph pyrimidine were established as isosteres of trans-cinnamide moiety. Applying this isosterism to previously reported p-arylthio cinnamides resulted in the identification of 4-amino-6-(p-arylthio)phenylpyrimidines and 2-amino-4-(p-arylthio)phenylpyridines I (X = N, CH, R1 = 2-Me2CH; X = CH, R1 = 2-MeO, 3,4-OCH2CH2O; R2R3N = pyrrolidinyl, 4-hydroxypiperidinyl, 4-formyl-1-piperazinyl, etc.) as potent antagonists of LFA-1/ICAM-1 binding.

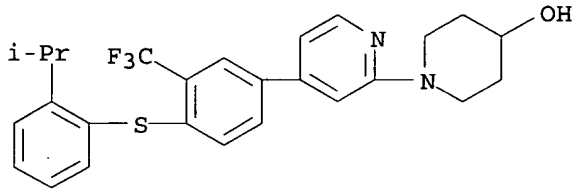
IT **388117-88-2P 388117-90-6P 388117-91-7P**
388117-93-9P 388117-94-0P 388117-96-2P
388117-97-3P 388117-98-4P 388117-99-5P
388118-00-1P 388118-02-3P 388118-06-7P
388118-07-8P 388118-08-9P 388118-09-0P
388118-11-4P 388118-12-5P 388118-14-7P
388118-15-8P 388118-16-9P 388118-17-0P
388118-18-1P 388118-20-5P 388118-22-7P
388118-24-9P 415718-12-6P 831189-91-4P
831189-92-5P 831189-93-6P 831189-94-7P
831189-95-8P 831189-96-9P 831189-97-0P
831189-98-1P 831189-99-2P 831190-00-2P
831190-01-3P 831190-02-4P 831190-04-6P
831190-07-9P 831190-09-1P 831190-10-4P
831190-11-5P 831190-12-6P 831190-13-7P
831190-14-8P 831190-15-9P 831190-16-0P
831190-17-1P 831190-18-2P 831190-19-3P
831190-20-6P 831190-21-7P 831190-22-8P
831190-23-9P 831190-24-0P 831190-25-1P
831190-26-2P 831190-27-3P 831190-28-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of amino-substituted arylthiophenyl oxazoles, thiazoles, pyridines and pyrimidines as isosteres of trans-cinnamides and potent antagonists of LFA-1/ICAM-1 binding)

RN 388117-88-2 HCAPLUS
CN 3-Pyrrolidinol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-

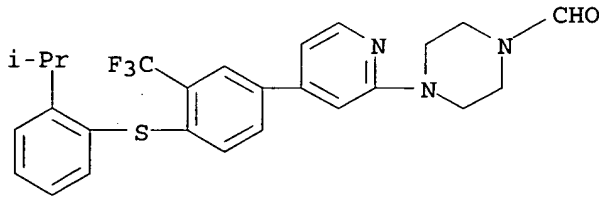
(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



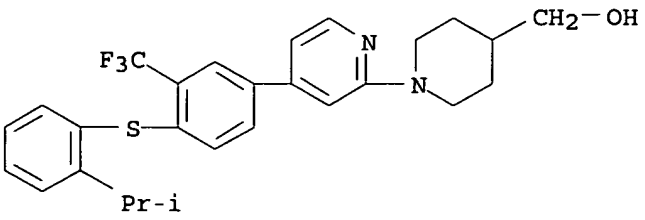
RN 388117-90-6 HCAPLUS
CN 4-Piperidinol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388117-91-7 HCAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

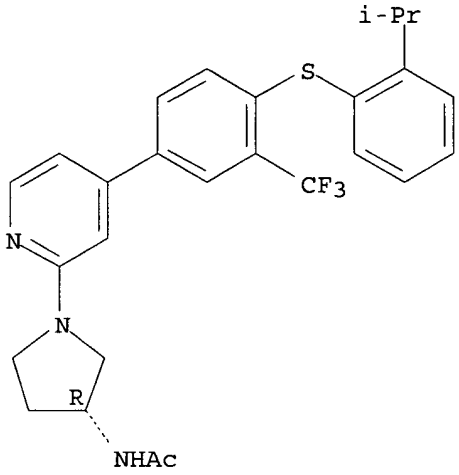


RN 388117-93-9 HCAPLUS
CN 4-Piperidinemethanol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

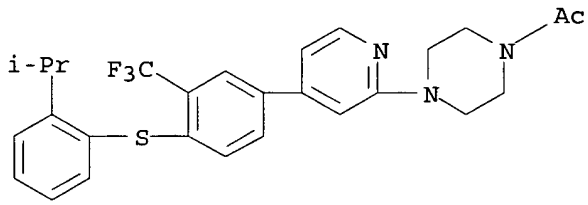


RN 388117-94-0 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

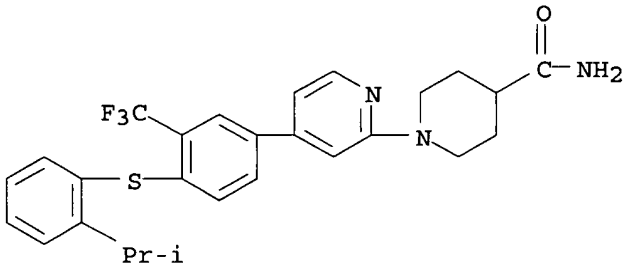
Absolute stereochemistry.



RN 388117-96-2 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

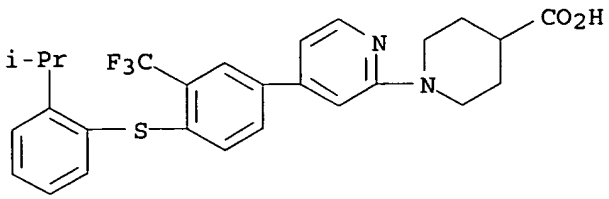


RN 388117-97-3 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

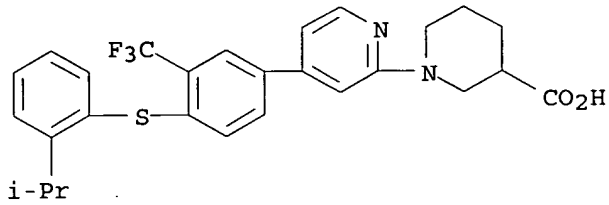


RN 388117-98-4 HCAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-

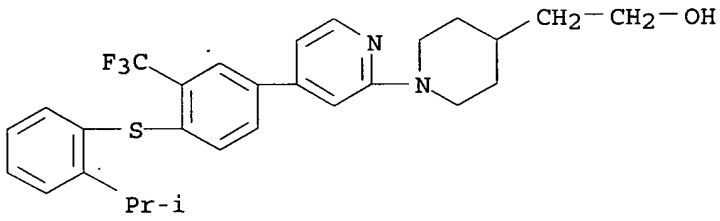
(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388117-99-5 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

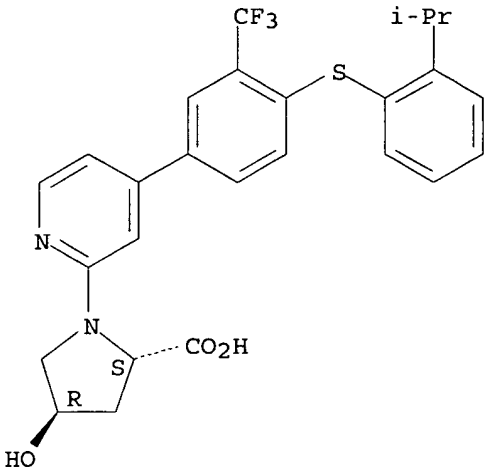


RN 388118-00-1 HCAPLUS
CN 4-Piperidineethanol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



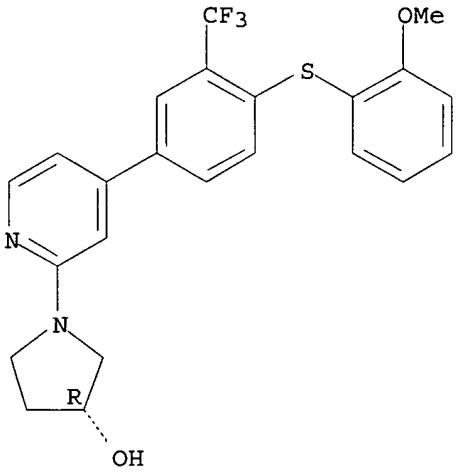
RN 388118-02-3 HCAPLUS
CN L-Proline, 4-hydroxy-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



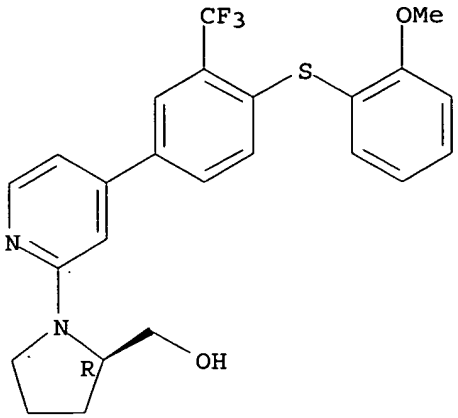
RN 388118-06-7 HCAPLUS
CN 3-Pyrrolidinol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

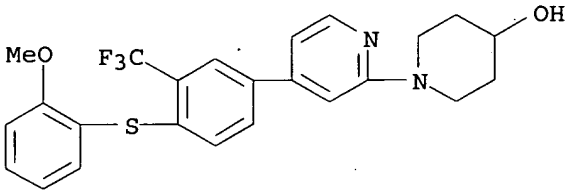


RN 388118-07-8 HCAPLUS
CN 2-Pyrrolidinemethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (2R)- (9CI) (CA INDEX NAME)

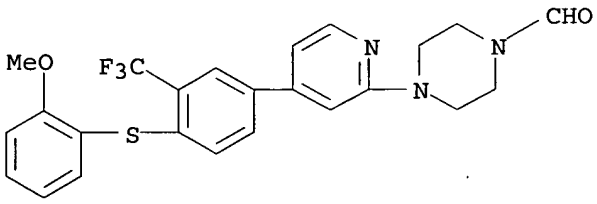
Absolute stereochemistry.



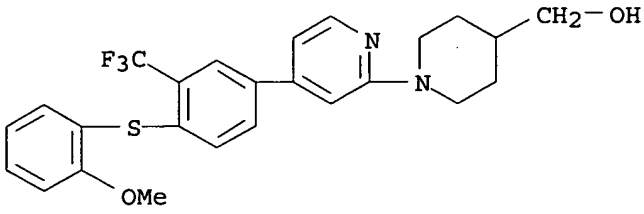
RN 388118-08-9 HCAPLUS
CN 4-Piperidinol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388118-09-0 HCAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

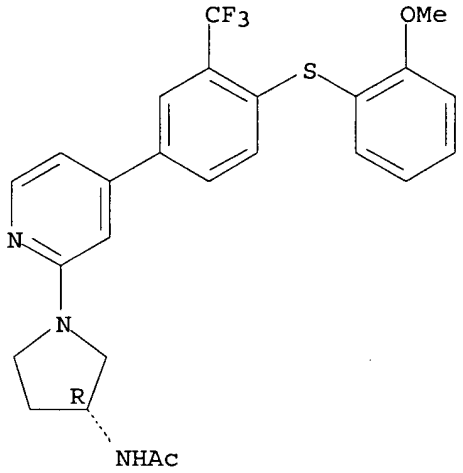


RN 388118-11-4 HCAPLUS
CN 4-Piperidinemethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

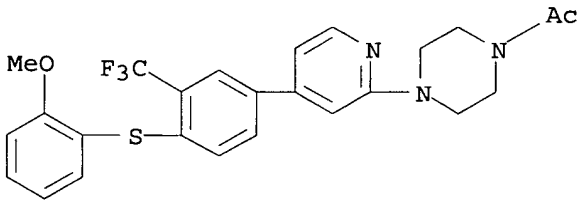


RN 388118-12-5 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

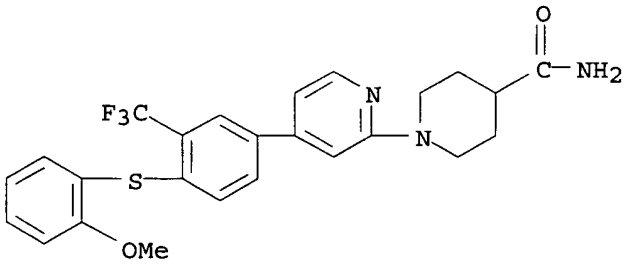
Absolute stereochemistry.



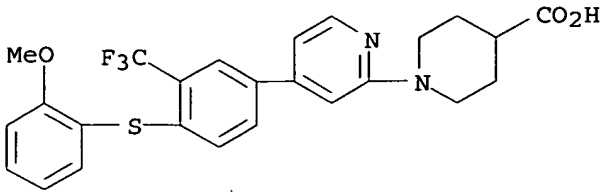
RN 388118-14-7 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



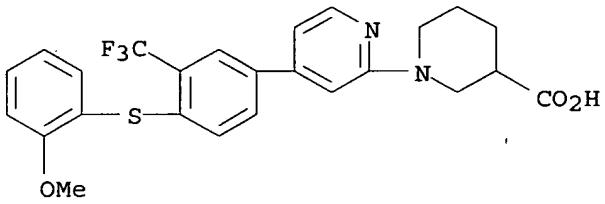
RN 388118-15-8 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



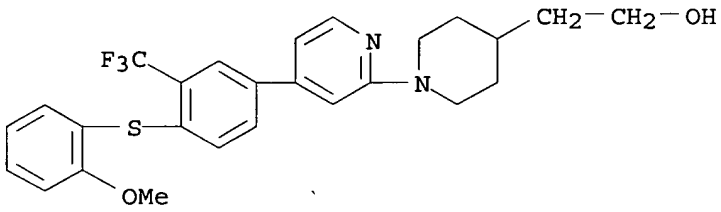
RN 388118-16-9 HCAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388118-17-0 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

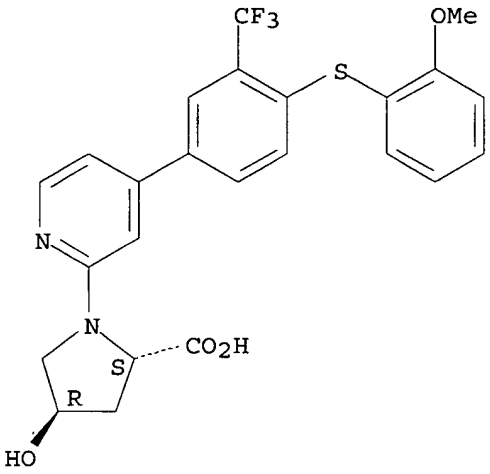


RN 388118-18-1 HCAPLUS
CN 4-Piperidineethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

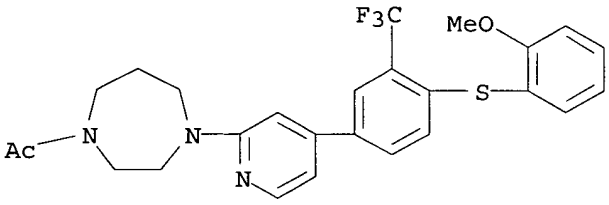


RN 388118-20-5 HCAPLUS
CN L-Proline, 4-hydroxy-1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

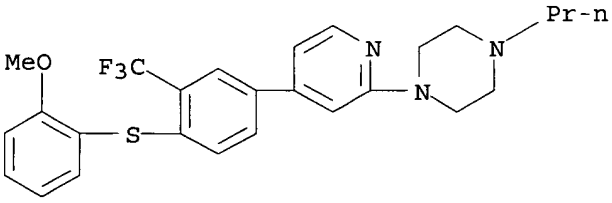
Absolute stereochemistry.



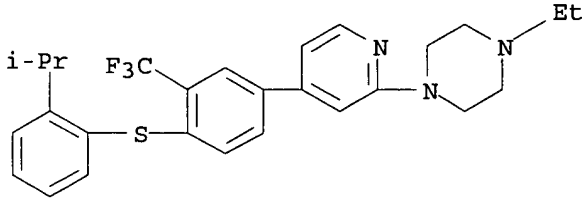
RN 388118-22-7 HCAPLUS
CN 1H-1,4-Diazepine, 1-acetylhexahydro-4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



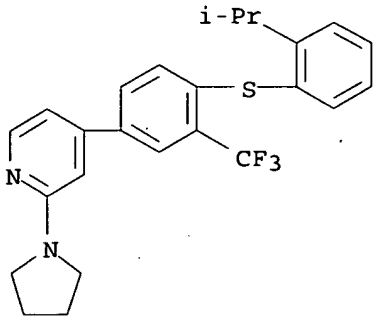
RN 388118-24-9 HCAPLUS
CN Piperazine, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-propyl- (9CI) (CA INDEX NAME)



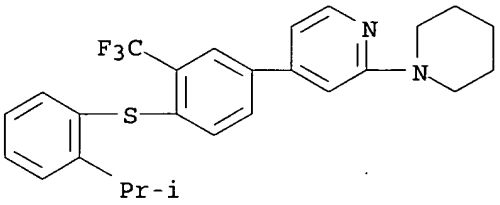
RN 415718-12-6 HCAPLUS
CN Piperazine, 1-ethyl-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



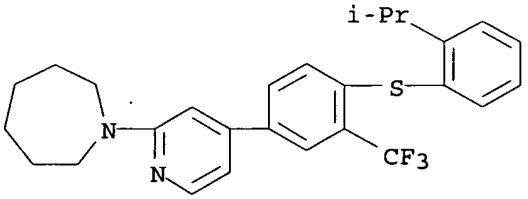
RN 831189-91-4 HCAPLUS
CN Pyridine, 4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



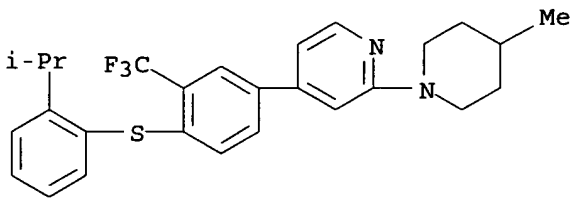
RN 831189-92-5 HCAPLUS
CN Pyridine, 4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-(1-piperidinyl)- (9CI) (CA INDEX NAME)



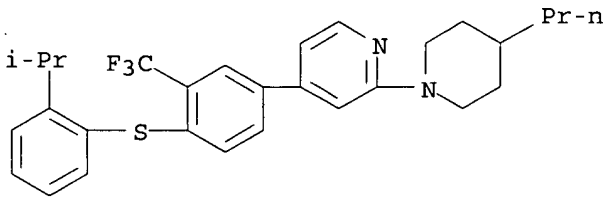
RN 831189-93-6 HCAPLUS
CN 1H-Azepine, hexahydro-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



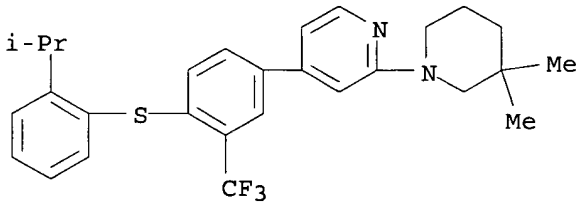
RN 831189-94-7 HCAPLUS
CN Pyridine, 4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 831189-95-8 HCAPLUS
CN Pyridine, 4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-(4-propyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

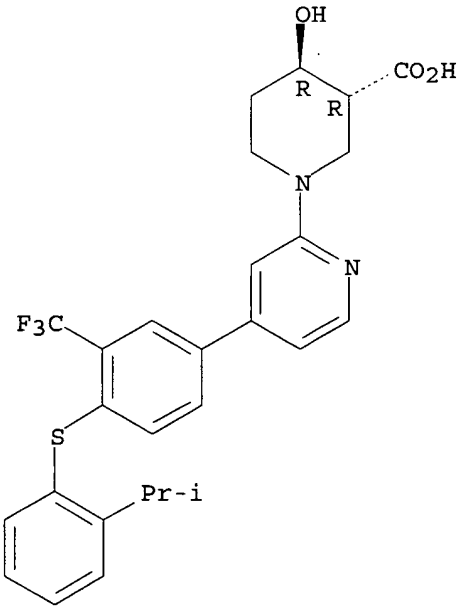


RN 831189-96-9 HCAPLUS
CN Pyridine, 2-(3,3-dimethyl-1-piperidinyl)-4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

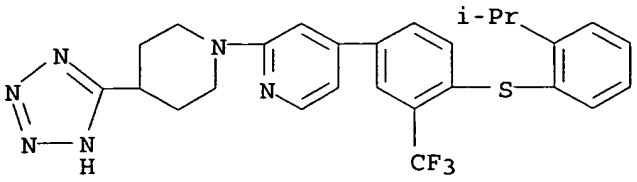


RN 831189-97-0 HCAPLUS
CN 3-Piperidinecarboxylic acid, 4-hydroxy-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

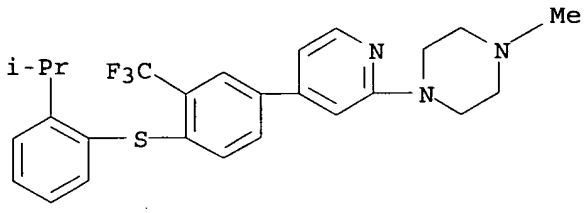
Relative stereochemistry.



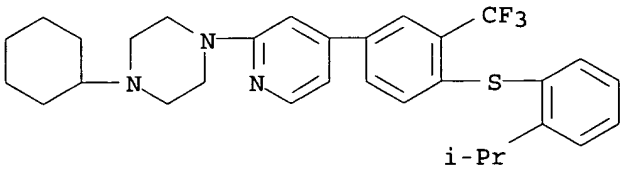
RN 831189-98-1 HCAPLUS
CN Pyridine, 4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-[4-(1H-tetrazol-5-yl)-1-piperidinyl]- (9CI) (CA INDEX NAME)



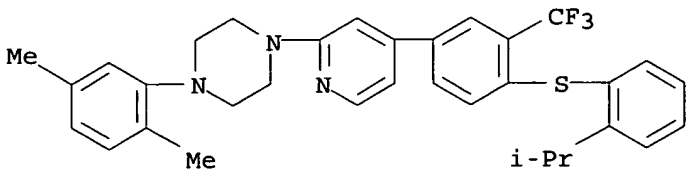
RN 831189-99-2 HCAPLUS
CN Piperazine, 1-methyl-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



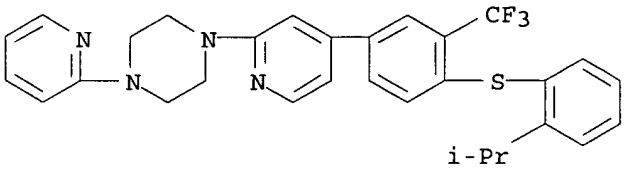
RN 831190-00-2 HCAPLUS
CN Piperazine, 1-cyclohexyl-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



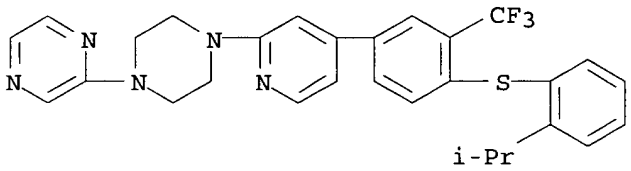
RN 831190-01-3 HCAPLUS
CN Piperazine, 1-(2,5-dimethylphenyl)-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 831190-02-4 HCAPLUS
CN Piperazine, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)

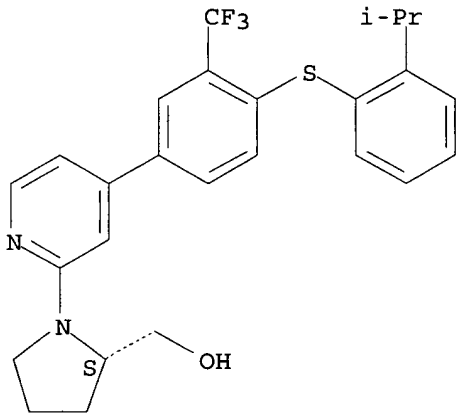


RN 831190-04-6 HCAPLUS
CN Pyrazine, [4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)



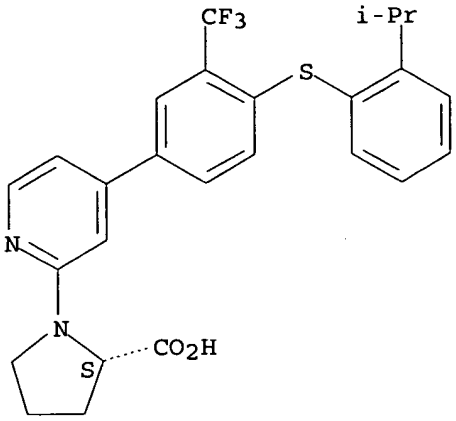
RN 831190-07-9 HCAPLUS
CN 2-Pyrrolidinemethanol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



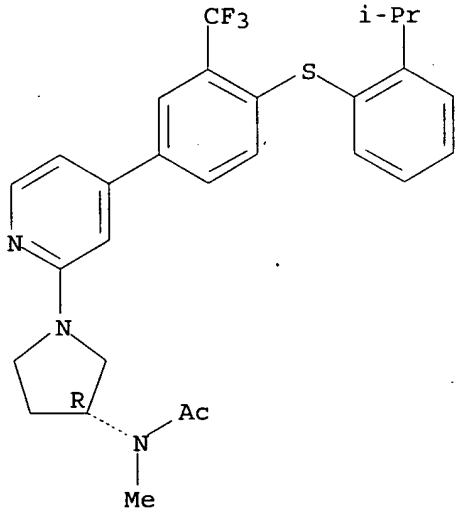
RN 831190-09-1 HCAPLUS
CN L-Proline, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



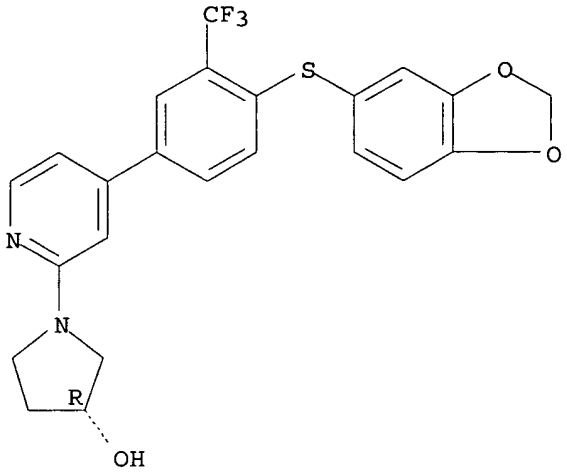
RN 831190-10-4 HCAPLUS
CN Acetamide, N-methyl-N-[(3R)-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



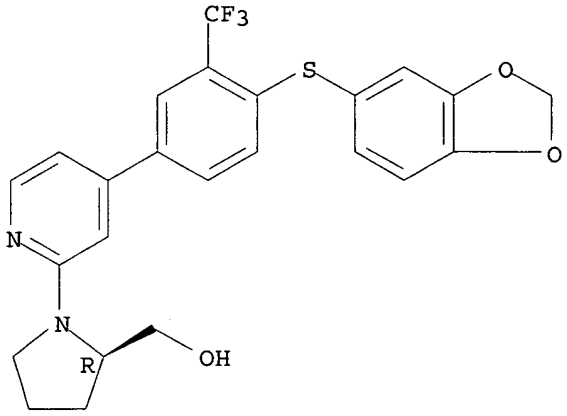
RN 831190-11-5 HCAPLUS
CN 3-Pyrrolidinol, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



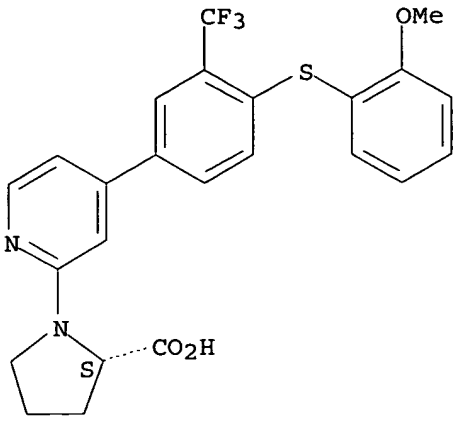
RN 831190-12-6 HCAPLUS
CN 2-Pyrrolidinemethanol, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



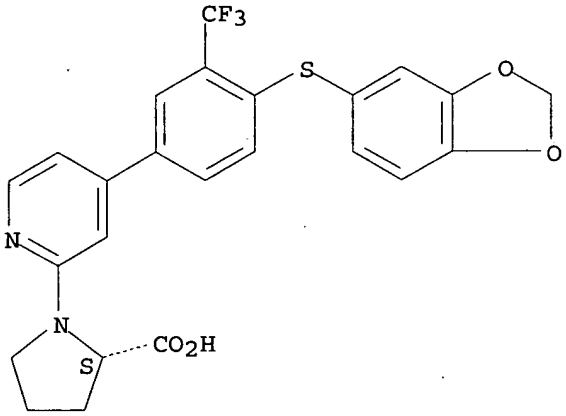
RN 831190-13-7 HCAPLUS
CN L-Proline, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



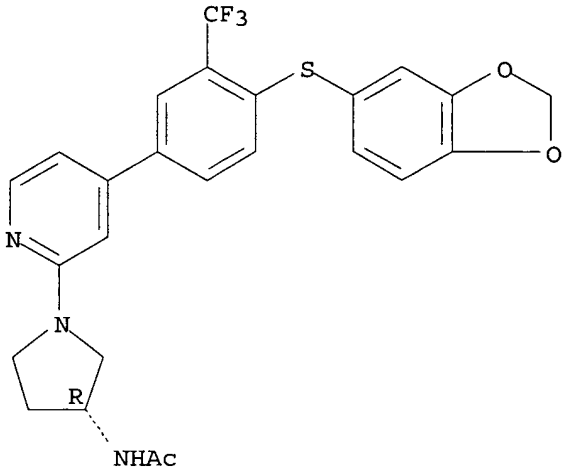
RN 831190-14-8 HCAPLUS
CN L-Proline, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



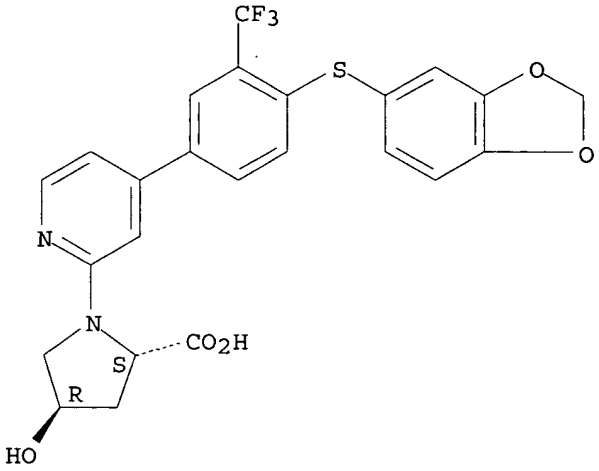
RN 831190-15-9 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



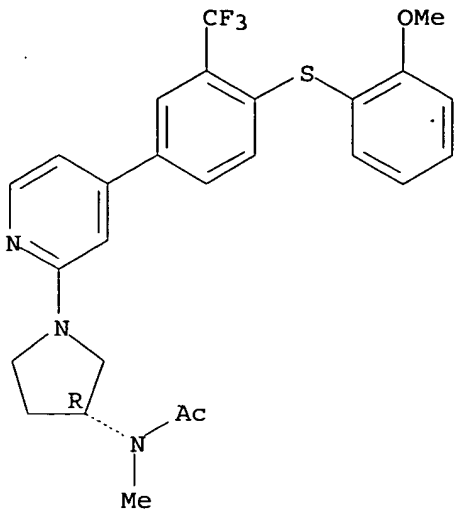
RN 831190-16-0 HCAPLUS
CN L-Proline, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-hydroxy-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



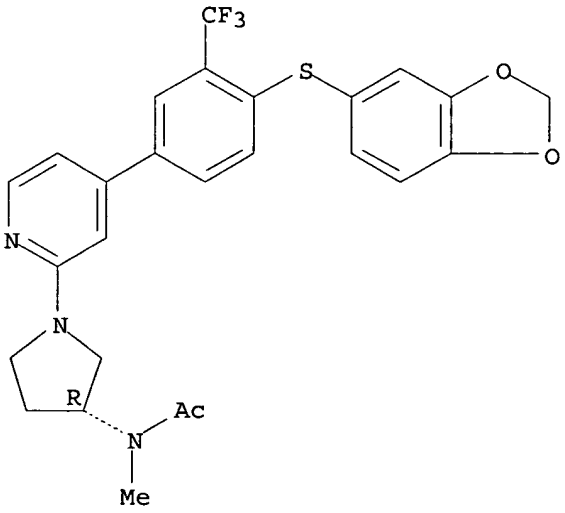
RN 831190-17-1 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

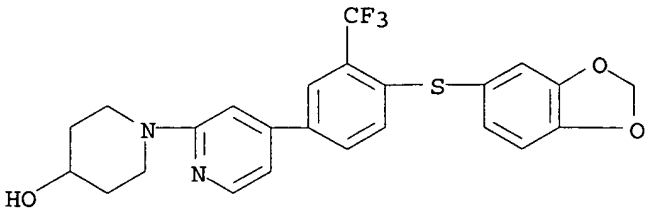


RN 831190-18-2 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]-N-methyl- (9CI) (CA INDEX NAME)

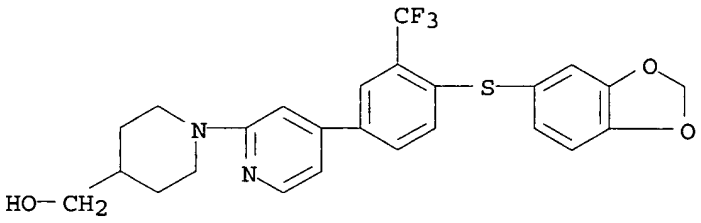
Absolute stereochemistry.



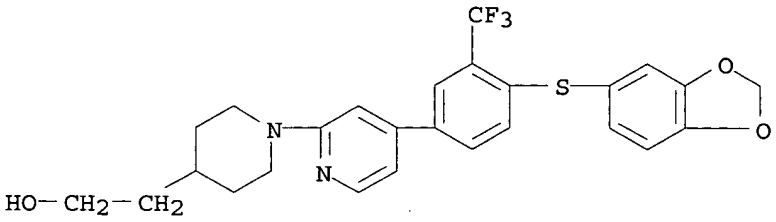
RN 831190-19-3 HCAPLUS
CN 4-Piperidinol, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



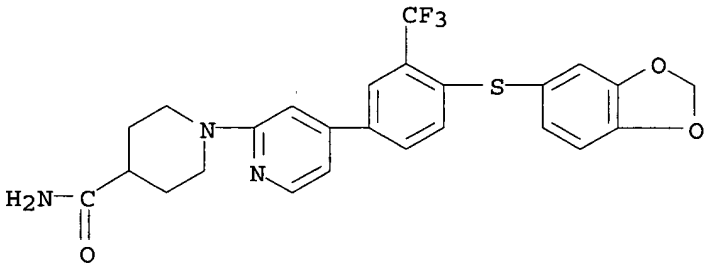
RN 831190-20-6 HCAPLUS
CN 4-Piperidinemethanol, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 831190-21-7 HCAPLUS
CN 4-Piperidineethanol, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

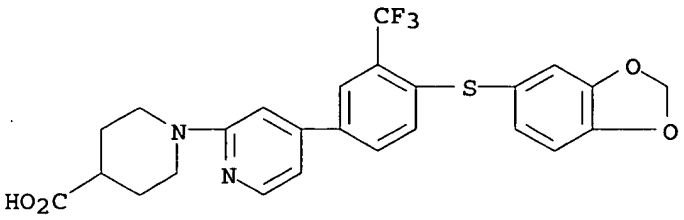


RN 831190-22-8 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

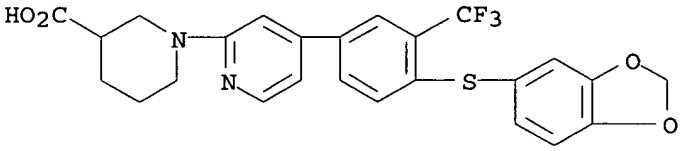


RN 831190-23-9 HCAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-

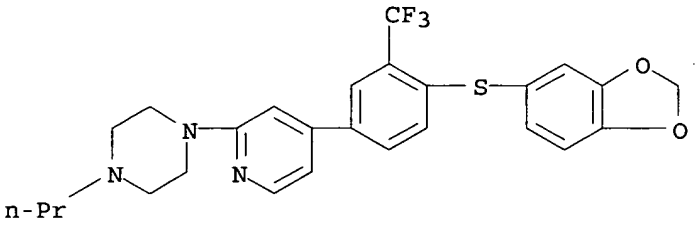
(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



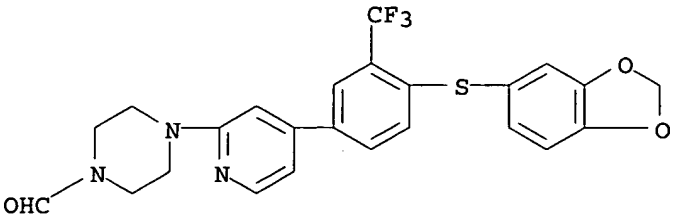
RN 831190-24-0 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



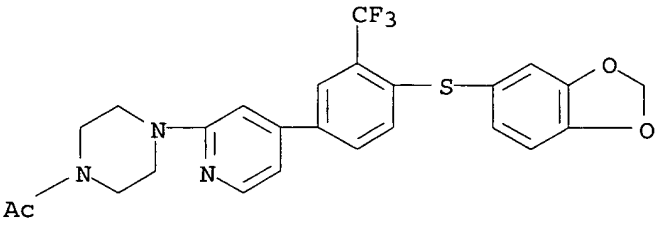
RN 831190-25-1 HCAPLUS
CN Piperazine, 1-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-propyl- (9CI) (CA INDEX NAME)



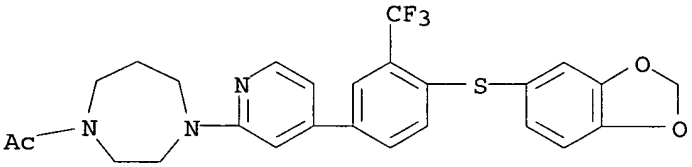
RN 831190-26-2 HCAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 831190-27-3 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

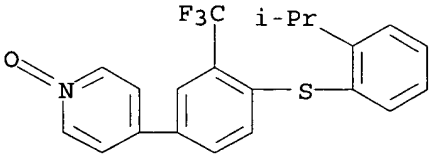


RN 831190-28-4 HCAPLUS
CN 1H-1,4-Diazepine, 1-acetyl-4-[4-[4-(1,3-benzodioxol-5-ylthio)-3-(trifluoromethyl)phenyl]-2-pyridinyl]hexahydro- (9CI) (CA INDEX NAME)

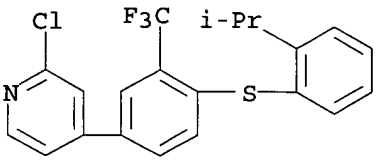


IT **388118-61-4P 388118-62-5P 388118-65-8P 388118-66-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino-substituted arylthiophenyl oxazoles, thiazoles, pyridines and pyrimidines as isosteres of trans-cinnamides and potent antagonists of LFA-1/ICAM-1 binding)

RN 388118-61-4 HCAPLUS
CN Pyridine, 4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-, 1-oxide (9CI) (CA INDEX NAME)

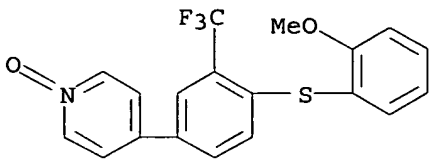


RN 388118-62-5 HCAPLUS
CN Pyridine, 2-chloro-4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

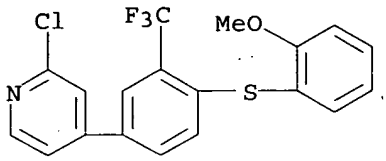


RN 388118-65-8 HCAPLUS
CN Pyridine, 4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-,

1-oxide (9CI) (CA INDEX NAME)



RN 388118-66-9 HCAPLUS
CN Pyridine, 2-chloro-4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



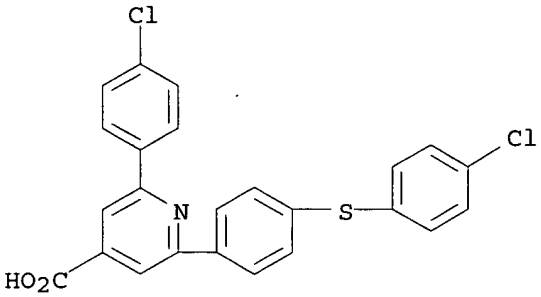
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1019618 HCAPLUS
DOCUMENT NUMBER: 142:69141
TITLE: Methods of identifying non-specific inhibitors of biomolecules
INVENTOR(S): Shoichet, Brian K.; McGovern, Susan L.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 16 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004234942	A1	20041125	US 2002-171814		20020614
PRIORITY APPLN. INFO.:			US 2001-298527P	P	20010615

AB The invention provides methods of identifying compds. that non-specifically inhibit biol. reactions. The invention further includes kits that facilitate this identification. In addition, compilations of compds. for use in high throughput drug screening that have been evaluated by the disclosed methodol. are also part of the d invention. The invention provides methods for identifying a false pos. in a screening assay by measuring the activity of at least one biol. activity in the presence and absence of a small mol. compound capable of inhibiting aggregate formation, e.g., digitonin.
IT **813420-78-9**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(methods of identifying non-specific inhibitors of biomols.)
RN 813420-78-9 HCAPLUS

CN 4-Pyridinecarboxylic acid, 2-(4-chlorophenyl)-6-[4-[(4-chlorophenyl)thio]phenyl]- (9CI) (CA INDEX NAME)



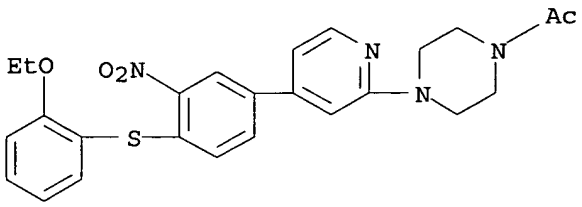
L12 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:121178 HCAPLUS
DOCUMENT NUMBER: 140:299089
TITLE: Structure of an Allosteric Inhibitor of LFA-1 Bound to the I-Domain Studied by Crystallography, NMR, and Calorimetry
AUTHOR(S): Crump, Matthew P.; Ceska, Thomas A.; Spyracopoulos, Leo; Henry, Alistair; Archibald, Sarah C.; Alexander, Rikki; Taylor, Richard J.; Findlow, Stuart C.; O'Connell, James; Robinson, Martyn K.; Shock, Anthony
CORPORATE SOURCE: School of Biological Sciences, University of Southampton, Southampton, SO16 7PX, UK
SOURCE: Biochemistry (2004), 43(9), 2394-2404
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB LFA-1 (lymphocyte function-associated antigen-1) plays a role in intercellular adhesion and lymphocyte trafficking and activation and is an attractive anti-inflammatory drug target. The α-subunit of LFA-1, in common with several other integrins, has an N-terminally inserted domain (I-domain) of .apprx.200 amino acids that plays a central role in regulating ligand binding to LFA-1. An addnl. region, termed the I-domain allosteric site (IDAS), has been identified exclusively within the LFA-1 I-domain and shown to regulate the function of this protein. The IDAS is occupied by small mol. LFA-1 inhibitors when cocrystd. or analyzed by 15N-1H HSQC (heteronuclear single-quantum coherence) NMR titration expts. We report here a novel arylthio inhibitor that binds the I-domain with a Kd of 18.3 nM as determined by isothermal titration calorimetry (ITC). This value is in close agreement with the IC50 (10.9 nM) derived from a biochem. competition assay (DELFIA) that measures the level of inhibition of binding of whole LFA-1 to its ligand, ICAM-1. Having established the strong affinity of the arylthio inhibitor for the isolated I-domain, we have used a range of techniques to further characterize the binding, including ITC, NMR, and X-ray crystallog. We have first developed an effective ITC binding assay for use with low-solubility inhibitors that avoids the need for ELISA-based assays. In addition, we utilized a fast NMR-based assay for the generation of I-domain-inhibitor models. This is based around the collection of HCCH-TOCSY spectra of LFA-1 in the bound form and the identification of a subset of side chain Me groups that give chemical

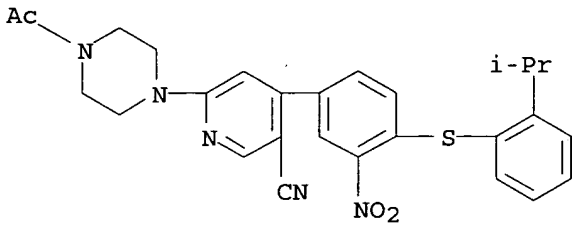
shift changes upon binding of LFA-1 inhibitors. This subset was used in two-dimensional 13C-15N and 15N-filtered and -edited two-dimensional NMR expts. to identify a minimal set of intraligand and ligand-protein NOEs, resp. (nuclear Overhauser enhancements). Models from the NMR data were assessed by comparison to an X-ray crystallog. structure of the complex, confirming that the method correctly predicted the essential features of the bound ligand.

IT **677009-29-9D**, complexes with LFA-1 **677009-30-2D**,
complexes with LFA-1
RL: PRP (Properties)
(crystallog., NMR, and calorimetry address interaction of allosteric inhibitors with I-domain of human LFA-1)

RN 677009-29-9 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-[(2-ethoxyphenyl)thio]-3-nitrophenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 677009-30-2 HCAPLUS
CN Piperazine, 1-acetyl-4-[5-cyano-4-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



own work

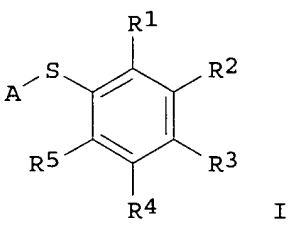
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:717059 HCAPLUS
DOCUMENT NUMBER: 137:247710
TITLE: Preparation of aryl phenylheterocyclyl sulfides as cell adhesion-inhibiting anti-inflammatory and immune-suppressive agents
INVENTOR(S): Wang, Gary T.; Wang, Sheldon; Gentles, Robert
PATENT ASSIGNEE(S): Icos Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 44 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

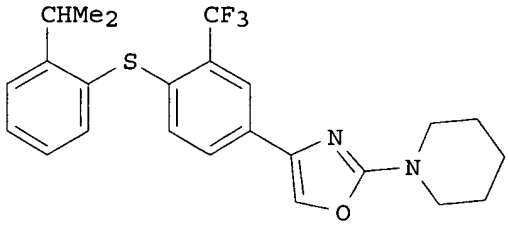
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2002132807	A1	20020919	US 2001-888840		20010625
US 6787542	B2	20040907			
US 2005014746	A1	20050120	US 2004-773332		20040209
PRIORITY APPLN. INFO.:			US 2000-214983P	P	20000629
			US 2001-888840	A3	20010625

OTHER SOURCE(S): MARPAT 137:247710

GI



I



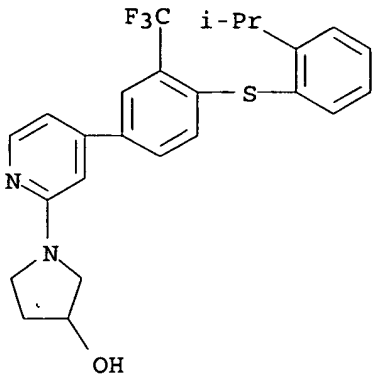
II

AB The title compds. [I; R1-R5 = H, halo, alkyl, etc. (with proviso that at least one of R1 or R3 = (un)substituted pyridyl, pyrimidyl, oxazolyl, etc.); A = (un)substituted aryl, heterocyclyl] were prepared for treating inflammatory and immune diseases, such as arthritis, asthma, reperfusion injury, inflammatory bowel disease etc. The products I had IC50 <20 μM for inhibition of ICAM-1 binding to LFA-1. 2-Me2CHC6H4SH was etherified with 4,3-F(F3C)C6H3COMe, followed by bromination, and reaction with 1-carbamoylpiperidine to give the sulfide II.

IT **388117-88-2P 388117-89-3P 388117-90-6P**
388117-91-7P 388117-92-8P 388117-93-9P
388117-94-0P 388117-95-1P 388117-96-2P
388117-97-3P 388117-98-4P 388117-99-5P
388118-00-1P 388118-01-2P 388118-02-3P
388118-03-4P 388118-04-5P 388118-05-6P
388118-06-7P 388118-07-8P 388118-08-9P
388118-09-0P 388118-10-3P 388118-11-4P
388118-12-5P 388118-13-6P 388118-14-7P
388118-15-8P 388118-16-9P 388118-17-0P
388118-18-1P 388118-19-2P 388118-20-5P
388118-21-6P 388118-22-7P 388118-23-8P
388118-24-9P 388118-25-0P 388118-26-1P
388118-27-2P 388118-28-3P 388118-29-4P
388118-30-7P 388118-31-8P 388118-32-9P
388118-33-0P 388118-34-1P 388118-35-2P
388118-36-3P 388118-37-4P 388118-38-5P
388118-39-6P 388118-40-9P 388118-41-0P
388118-42-1P 388118-43-2P 388118-44-3P
388118-45-4P 388118-46-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl phenylheterocyclyl sulfides as cell adhesion-inhibiting antiinflammatory and immunosuppressive agents)

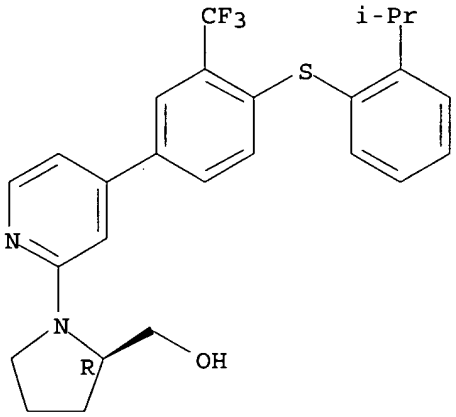
RN 388117-88-2 HCAPLUS

CN 3-Pyrrolidinol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

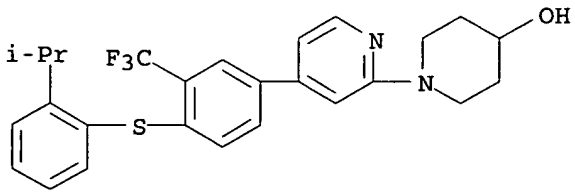


RN 388117-89-3 HCAPLUS
CN 2-Pyrrolidinemethanol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (2R)- (9CI) (CA INDEX NAME)

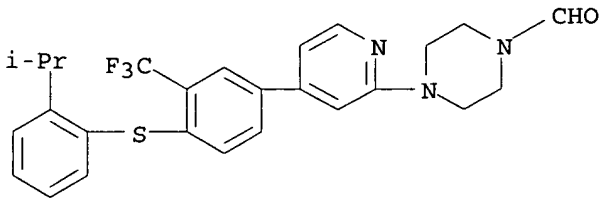
Absolute stereochemistry.



RN 388117-90-6 HCAPLUS
CN 4-Piperidinol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

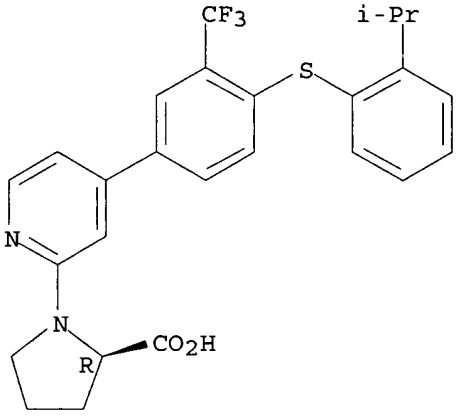


RN 388117-91-7 HCAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

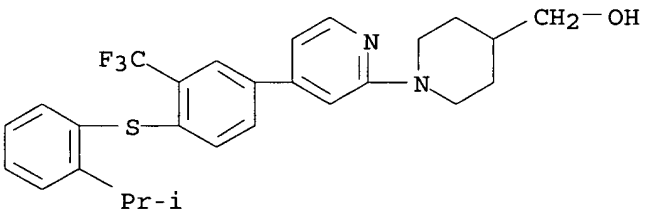


RN 388117-92-8 HCAPLUS
CN D-Proline, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

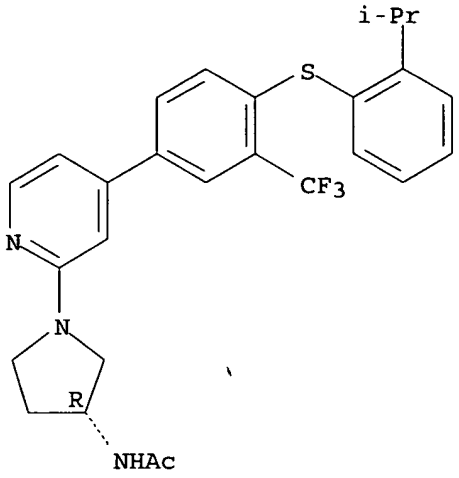


RN 388117-93-9 HCAPLUS
CN 4-Piperidinemethanol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

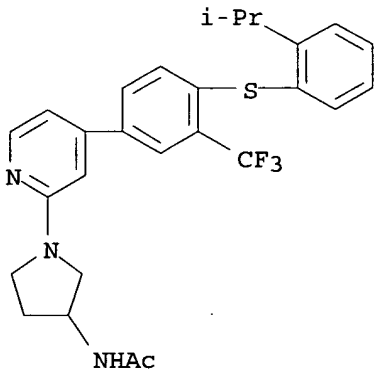


RN 388117-94-0 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

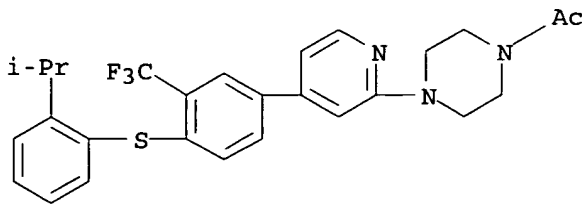
Absolute stereochemistry.



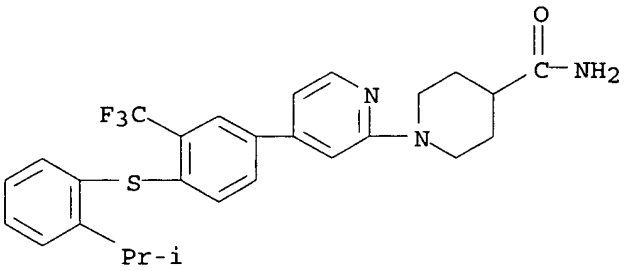
RN 388117-95-1 HCAPLUS
CN Acetamide, N-[1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)



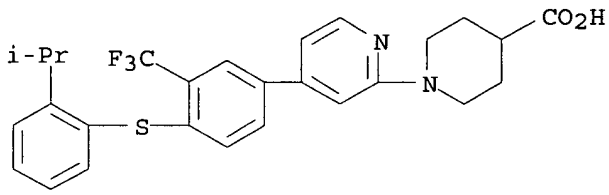
RN 388117-96-2 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



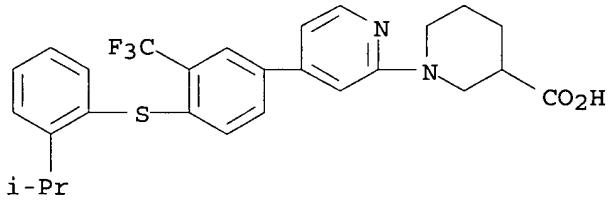
RN 388117-97-3 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



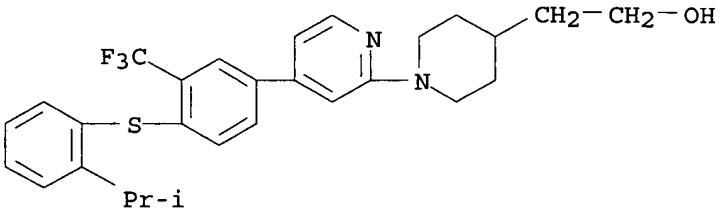
RN 388117-98-4 HCAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388117-99-5 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

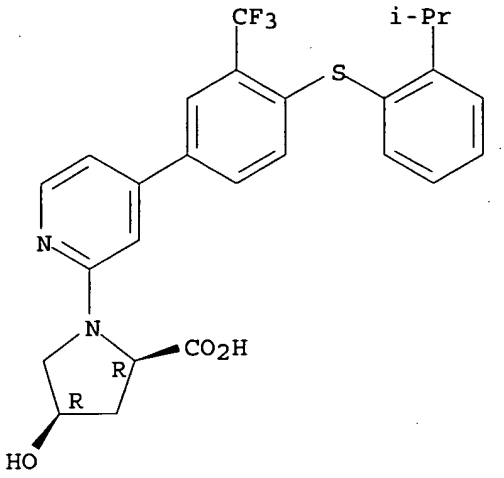


RN 388118-00-1 HCAPLUS
CN 4-Piperidineethanol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



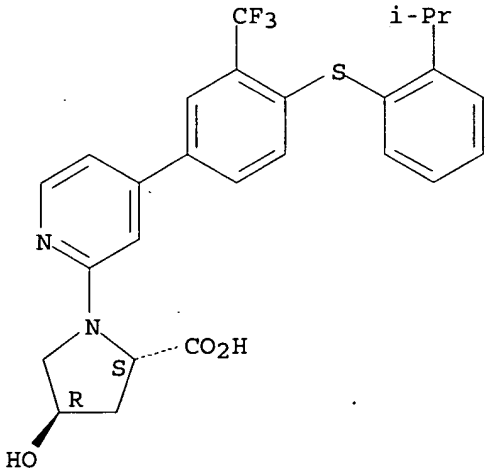
RN 388118-01-2 HCAPLUS
CN D-Proline, 4-hydroxy-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

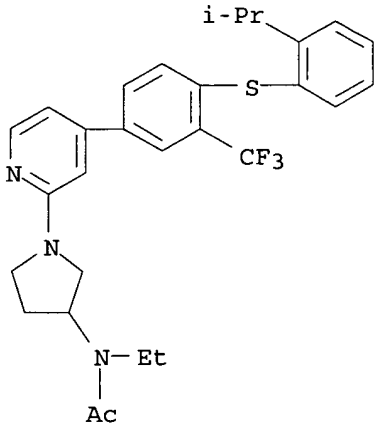


RN 388118-02-3 HCAPLUS
CN L-Proline, 4-hydroxy-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

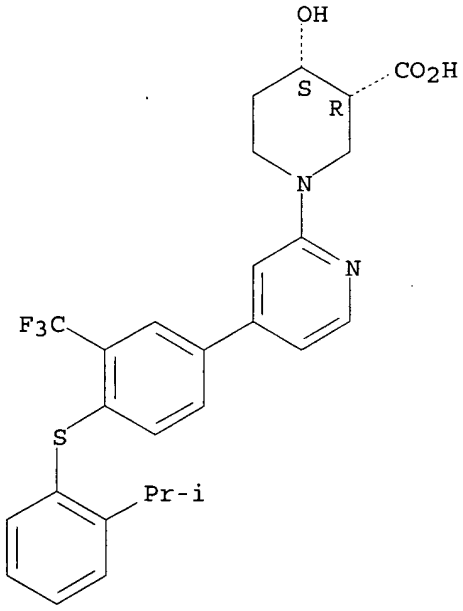


RN 388118-03-4 HCAPLUS
CN Acetamide, N-ethyl-N-[1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

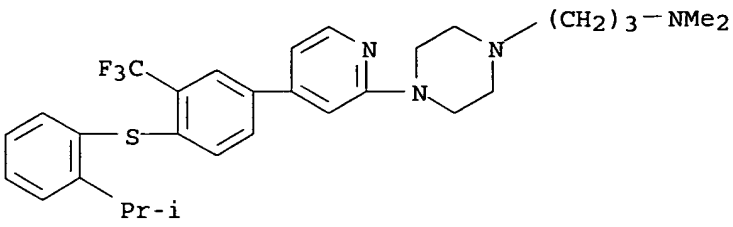


RN 388118-04-5 HCAPLUS
CN 3-Piperidinecarboxylic acid, 4-hydroxy-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

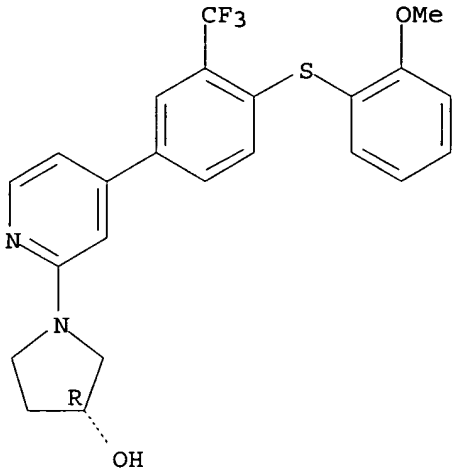


RN 388118-05-6 HCAPLUS
CN 1-Piperazinepropanamine, N,N-dimethyl-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



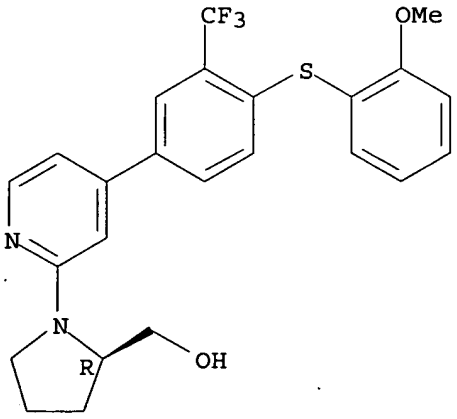
RN 388118-06-7 HCAPLUS
CN 3-Pyrrolidinol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



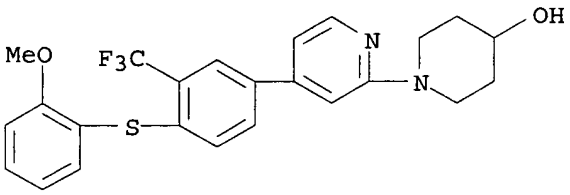
RN 388118-07-8 HCAPLUS
CN 2-Pyrrolidinemethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

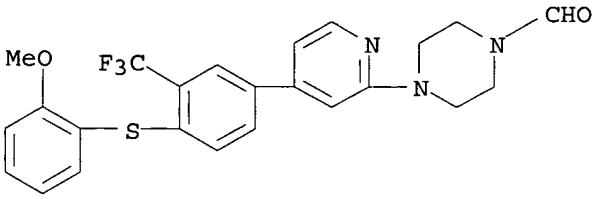


RN 388118-08-9 HCAPLUS

CN 4-Piperidinol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

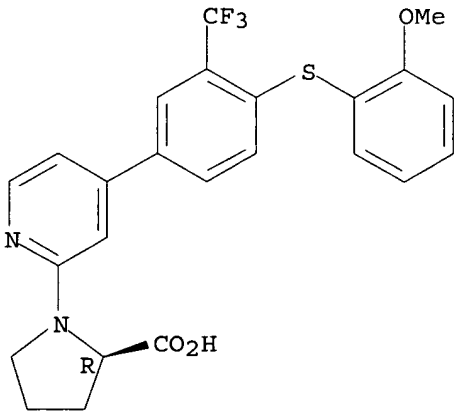


RN 388118-09-0 HCAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

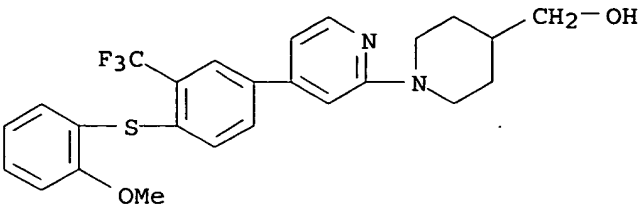


RN 388118-10-3 HCAPLUS
CN D-Proline, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

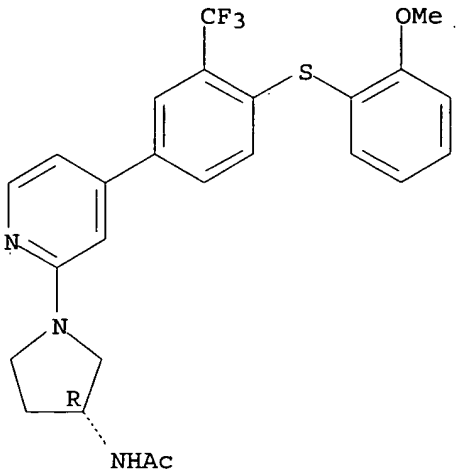


RN 388118-11-4 HCAPLUS
CN 4-Piperidinemethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

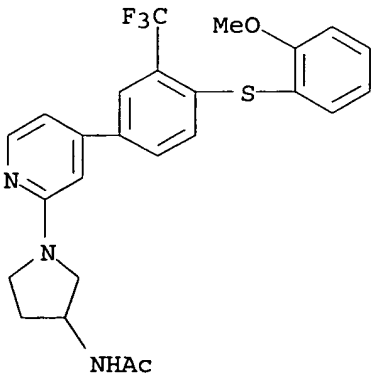


RN 388118-12-5 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

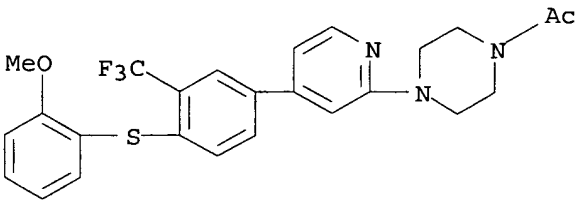
Absolute stereochemistry.



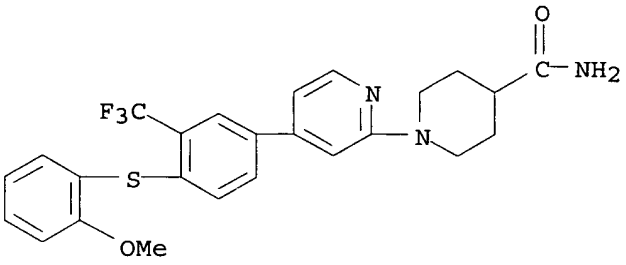
RN 388118-13-6 HCAPLUS
CN Acetamide, N-[1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)



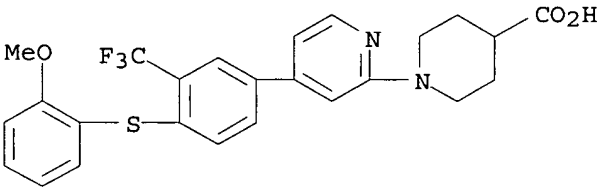
RN 388118-14-7 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



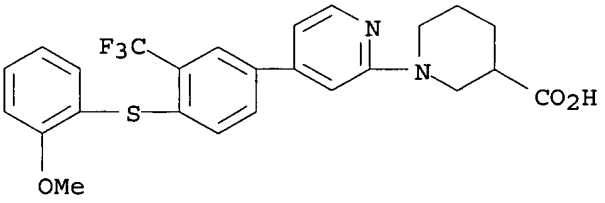
RN 388118-15-8 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



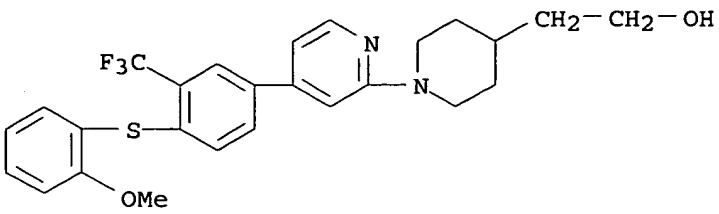
RN 388118-16-9 HCAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388118-17-0 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

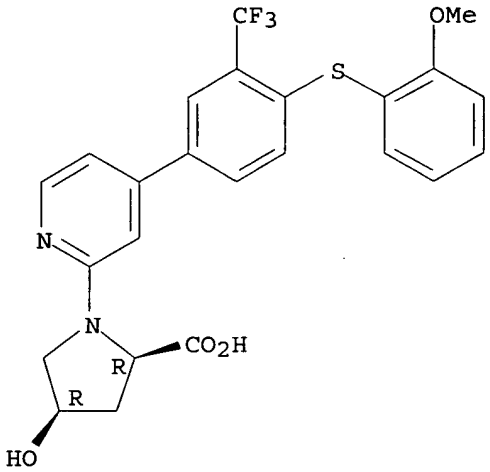


RN 388118-18-1 HCAPLUS
CN 4-Piperidineethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



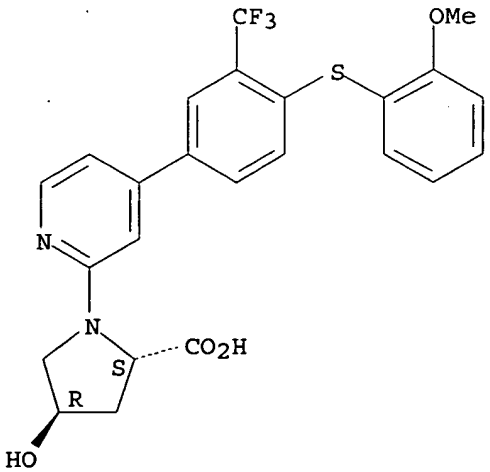
RN 388118-19-2 HCAPLUS
CN D-Proline, 4-hydroxy-1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

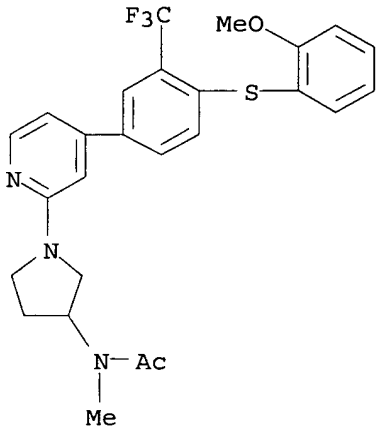


RN 388118-20-5 HCAPLUS
CN L-Proline, 4-hydroxy-1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

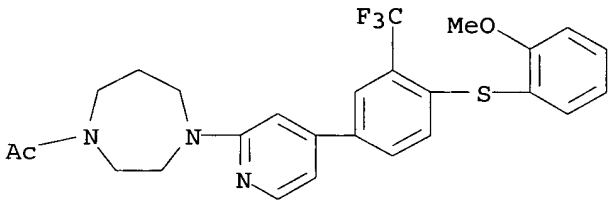
Absolute stereochemistry.



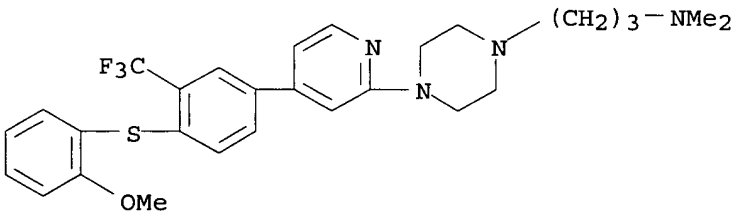
RN 388118-21-6 HCAPLUS
CN Acetamide, N-[1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]-N-methyl- (9CI) (CA INDEX NAME)



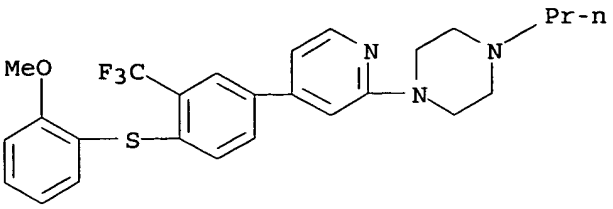
RN 388118-22-7 HCAPLUS
CN 1H-1,4-Diazepine, 1-acetylhexahydro-4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



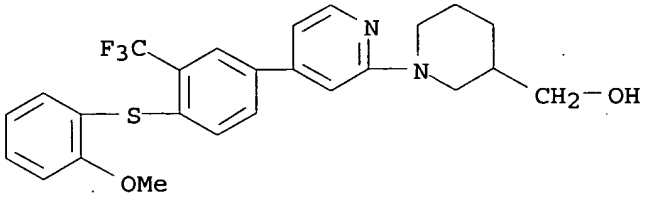
RN 388118-23-8 HCAPLUS
CN 1-Piperazinepropanamine, 4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 388118-24-9 HCAPLUS
CN Piperazine, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-propyl- (9CI) (CA INDEX NAME)

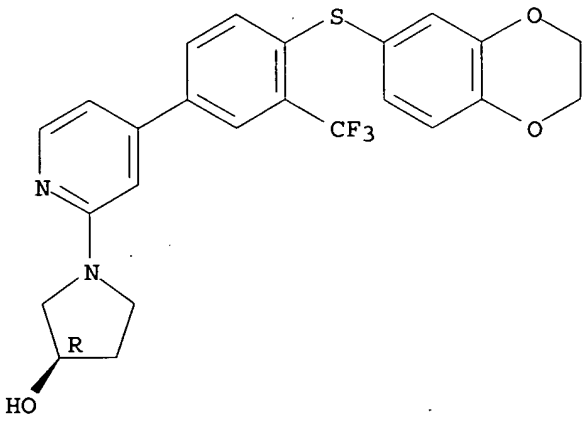


RN 388118-25-0 HCAPLUS
CN 3-Piperidinemethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

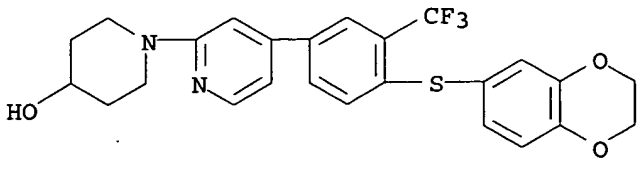


RN 388118-26-1 HCAPLUS
CN 3-Pyrrolidinol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

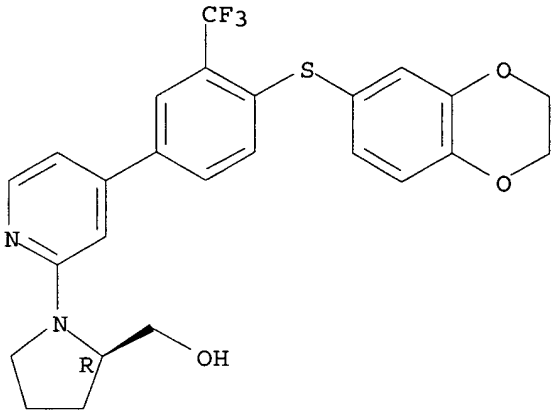


RN 388118-27-2 HCAPLUS
CN 4-Piperidinol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



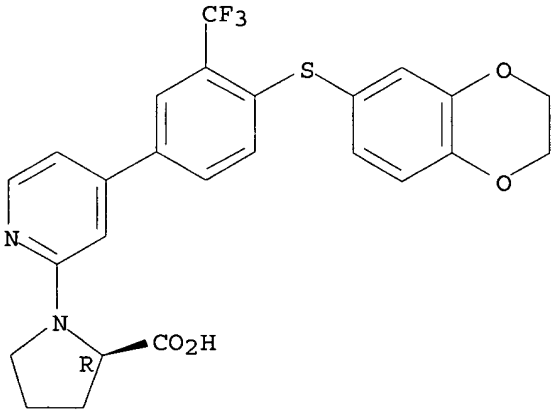
RN 388118-28-3 HCAPLUS
CN 2-Pyrrolidinemethanol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

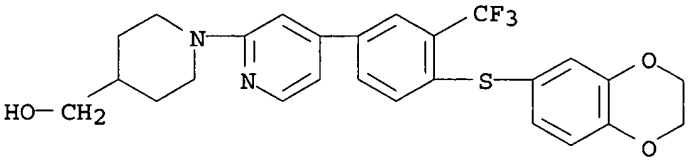


RN 388118-29-4 HCAPLUS
CN D-Proline, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

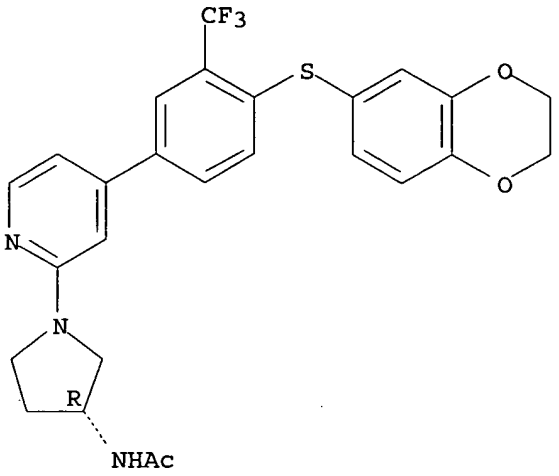


RN 388118-30-7 HCAPLUS
CN 4-Piperidinemethanol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

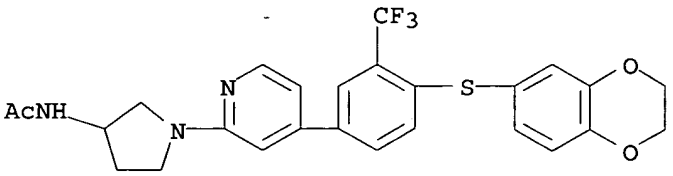


RN 388118-31-8 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

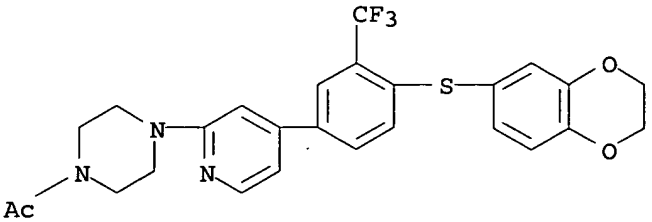
Absolute stereochemistry.



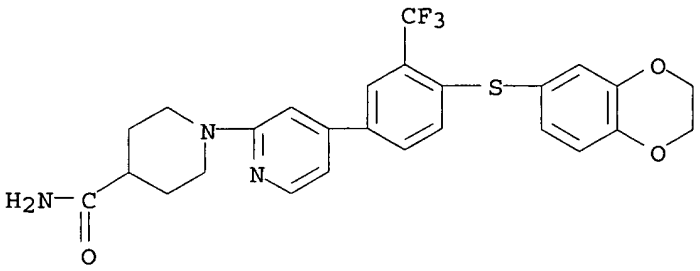
RN 388118-32-9 HCAPLUS
CN Acetamide, N-[1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)



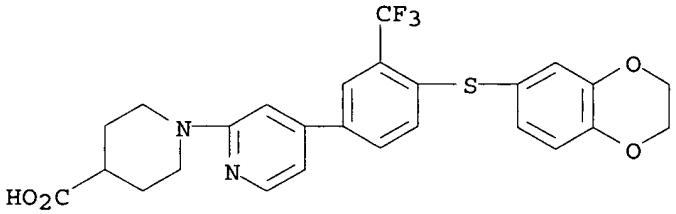
RN 388118-33-0 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



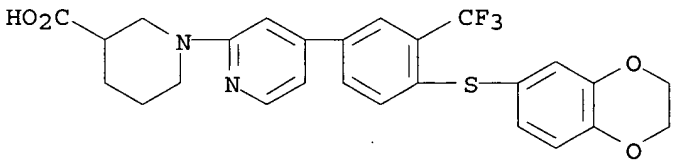
RN 388118-34-1 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



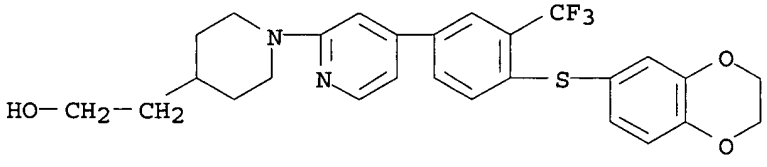
RN 388118-35-2 HCAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388118-36-3 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

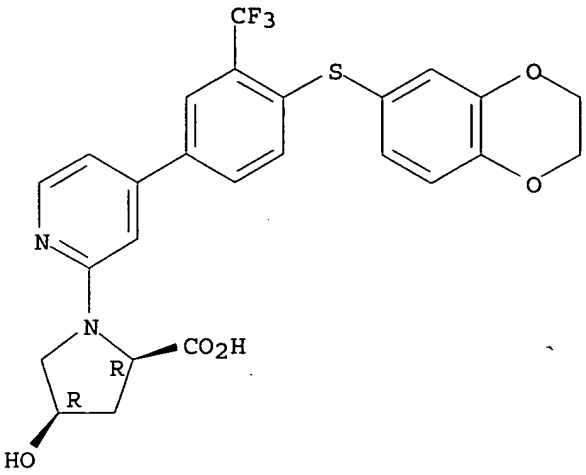


RN 388118-37-4 HCAPLUS
CN 4-Piperidineethanol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



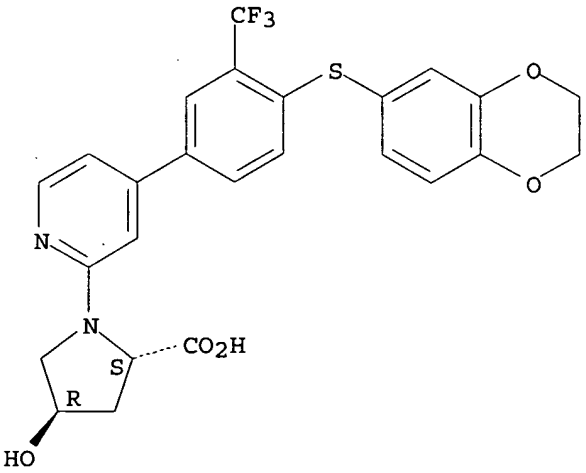
RN 388118-38-5 HCAPLUS
CN D-Proline, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-hydroxy-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

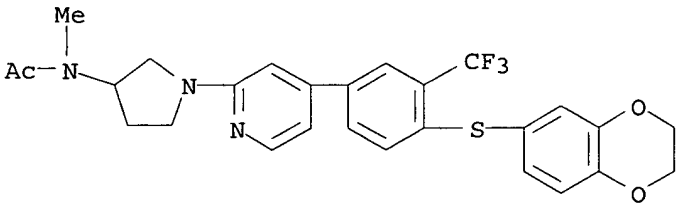


RN 388118-39-6 HCAPLUS
CN L-Proline, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-hydroxy-, (4R)- (9CI) (CA INDEX NAME)

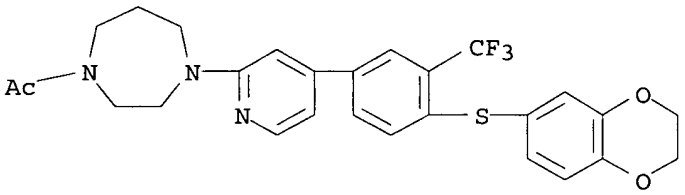
Absolute stereochemistry.



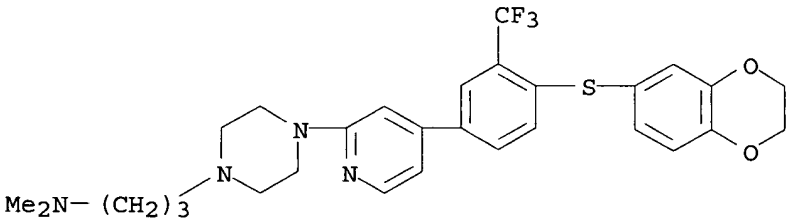
RN 388118-40-9 HCAPLUS
CN Acetamide, N-[1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]-N-methyl- (9CI) (CA INDEX NAME)



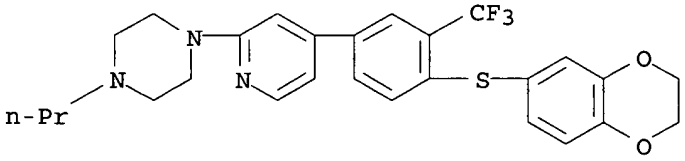
RN 388118-41-0 HCAPLUS
CN 1H-1,4-Diazepine, 1-acetyl-4-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]hexahydro- (9CI) (CA INDEX NAME)



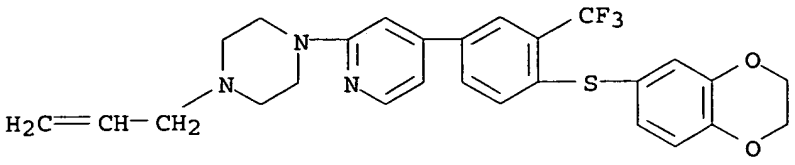
RN 388118-42-1 HCAPLUS
CN 1-Piperazinepropanamine, 4-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



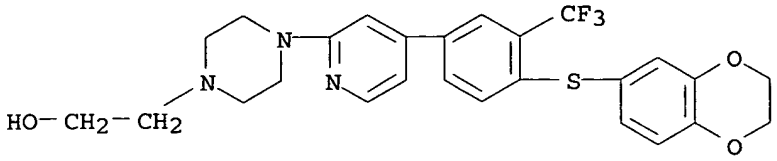
RN 388118-43-2 HCAPLUS
CN Piperazine, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-propyl- (9CI) (CA INDEX NAME)



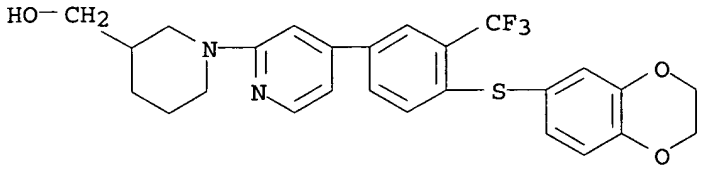
RN 388118-44-3 HCAPLUS
CN Piperazine, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-(2-propenyl)- (9CI) (CA INDEX NAME)



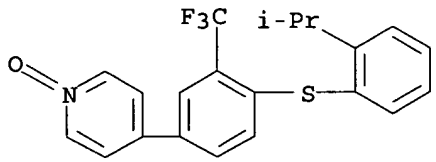
RN 388118-45-4 HCAPLUS
CN 1-Piperazineethanol, 4-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



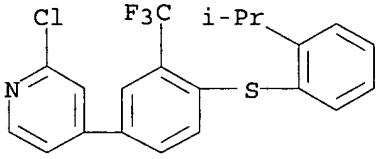
RN 388118-46-5 HCAPLUS
CN 3-Piperidinemethanol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



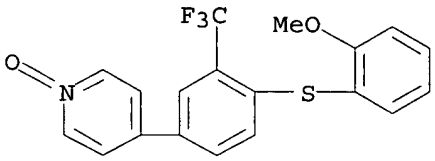
IT **388118-61-4P 388118-62-5P 388118-65-8P 388118-66-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl phenylheterocyclyl sulfides as cell adhesion-inhibiting antiinflammatory and immunosuppressive agents)
RN 388118-61-4 HCAPLUS
CN Pyridine, 4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-, 1-oxide (9CI) (CA INDEX NAME)



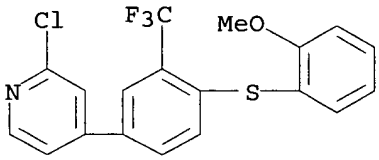
RN 388118-62-5 HCAPLUS
CN Pyridine, 2-chloro-4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 388118-65-8 HCAPLUS
CN Pyridine, 4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-, 1-oxide (9CI) (CA INDEX NAME)



RN 388118-66-9 HCAPLUS
CN Pyridine, 2-chloro-4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 111 THERE ARE 111 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:293978 HCAPLUS
DOCUMENT NUMBER: 136:337341
TITLE: Materials and methods to modulate ligand binding/enzymic activity of α/β proteins containing an allosteric regulatory site
INVENTOR(S): Stauton, Donald E.
PATENT ASSIGNEE(S): Icos Corporation, USA
SOURCE: PCT Int. Appl., 163 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002031511	A2	20020418	WO 2001-US32047	20011012
WO 2002031511	A3	20030313		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2425581	AA	20020418	CA 2001-2425581		20011012
AU 2002013196	A5	20020422	AU 2002-13196		20011012
US 2003088061	A1	20030508	US 2001-976935		20011012
EP 1325341	A2	20030709	EP 2001-981560		20011012
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004511496	T2	20040415	JP 2002-534845		20011012
PRIORITY APPLN. INFO.:			US 2000-239750P	P	20001012
			WO 2001-US32047	W	20011012

AB Methods of modulating binding between an α/β protein and a binding partner are provided, along with methods of identifying modulators and their use. The methods comprise contacting the α/β protein with an allosteric effector mol. which binds to an allosteric site of the α/β protein and alters the conformation of the α/β protein such that the binding of the α/β protein to a binding partner is modulated. Thus, a primary screen for inhibitors of the classical pathway complement protein C2 and alternative pathway complement protein factor B involving modifications of standard hemolytic CH50 and AH50 assays in a microtiter plate format was carried out. Lead compds. identified in this screen were submitted to a second screening using purified complement proteins to determine which stage of complement activation the compds. inhibited. Five diaryl sulfides were identified. Numerous other assays, e.g., to identify inhibitors of integrin αEβy interaction with E cadherin, inhibitors of Rac1 GDP-GTP exchange, or antagonists of E. coli 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase, were conducted as well.

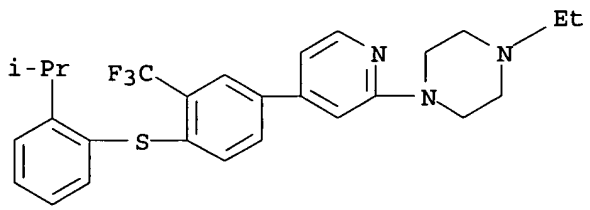
IT **415718-13-7**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(materials and methods to modulate ligand binding/enzymic activity of α/β proteins containing allosteric regulatory site)

RN 415718-13-7 HCAPLUS

CN Piperazine, 1-ethyl-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

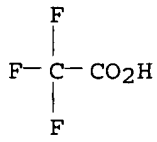
CM 1

CRN 415718-12-6
CMF C27 H30 F3 N3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

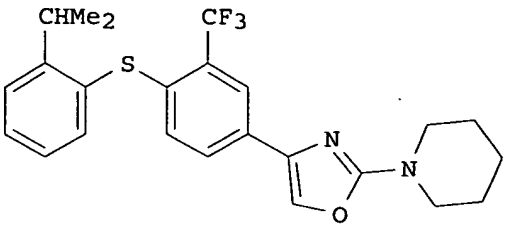


L12 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:31429 HCAPLUS
DOCUMENT NUMBER: 136:102394
TITLE: Aryl phenylheterocyclyl sulfide derivatives and their use as cell adhesion-inhibiting anti-inflammatory and immune-suppressive agents
INVENTOR(S): Wang, Gary T.; Wang, Sheldon; Gentles, Robert
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 135 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

same family

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002002539	A1	20020110	WO 2001-US20128	20010622
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2414461	AA	20020110	CA 2001-2414461	20010622
AU 2001068718	A5	20020114	AU 2001-68718	20010622
EP 1294704	A1	20030326	EP 2001-946705	20010622
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004502681	T2	20040129	JP 2002-507794	20010622
NZ 523445	A	20041029	NZ 2001-523445	20010622
PRIORITY APPLN. INFO.:			US 2000-606717 A	20000629
			US 2000-214983P P	20000629
			WO 2001-US20128 W	20010622

OTHER SOURCE(S): MARPAT 136:102394
GI

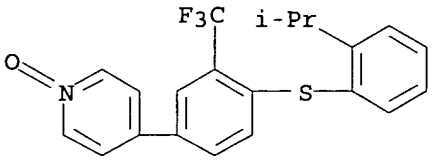


I

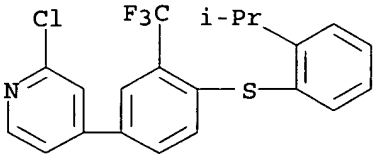
AB Title compds. were prepared for treating inflammatory and immune diseases, such as arthritis, asthma, reperfusion injury, inflammatory bowel disease etc. The products had IC50 <20 mM for inhibition of ICAM-1 binding to LFA-1. 2-Me2CHC6H4SHwas etherified with 4,3-F(F3C)C6H3COMe, followed by bromination, and reaction with 1-carbamoylpiperidine to give the sulfide I.

IT **388118-61-4P 388118-62-5P 388118-65-8P 388118-66-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl phenylheterocyclyl sulfides as cell adhesion-inhibiting antiinflammatory and immunosuppressive agents)

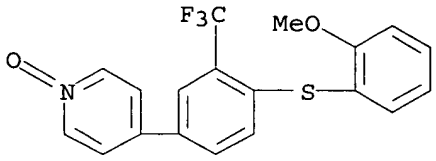
RN 388118-61-4 HCAPLUS
CN Pyridine, 4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-, 1-oxide (9CI) (CA INDEX NAME)



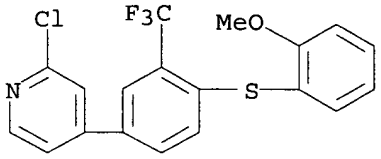
RN 388118-62-5 HCAPLUS
CN Pyridine, 2-chloro-4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 388118-65-8 HCAPLUS
CN Pyridine, 4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-, 1-oxide (9CI) (CA INDEX NAME)



RN 388118-66-9 HCAPLUS
CN Pyridine, 2-chloro-4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



IT **388117-88-2P 388117-89-3P 388117-90-6P**
388117-91-7P 388117-92-8P 388117-93-9P
388117-94-0P 388117-95-1P 388117-96-2P
388117-97-3P 388117-98-4P 388117-99-5P
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388118-03-4P 388118-04-5P 388118-05-6P
388118-06-7P 388118-07-8P 388118-08-9P
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388118-24-9P 388118-25-0P 388118-26-1P
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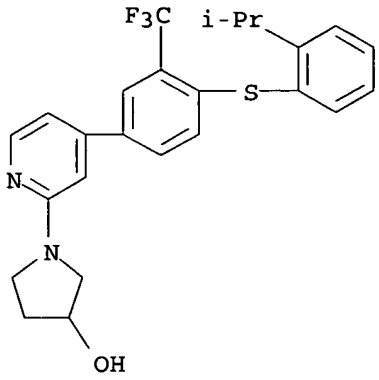
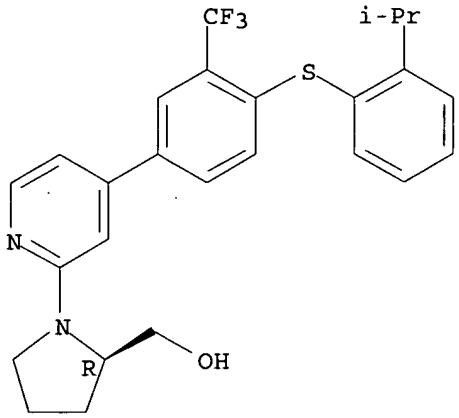
388118-30-7P 388118-31-8P 388118-32-9P
388118-33-0P 388118-34-1P 388118-35-2P
388118-36-3P 388118-37-4P 388118-38-5P
388118-39-6P 388118-40-9P 388118-41-0P
388118-42-1P 388118-43-2P 388118-44-3P
388118-45-4P 388118-46-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl phenylheterocyclyl sulfides as cell adhesion-inhibiting antiinflammatory and immunosuppressive agents)
RN 388117-88-2 HCAPLUS
CN 3-Pyrrolidinol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

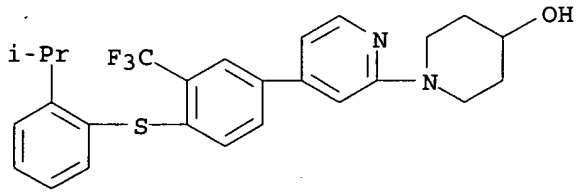


RN 388117-89-3 HCAPLUS
CN 2-Pyrrolidinemethanol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (2R)- (9CI) (CA INDEX NAME)

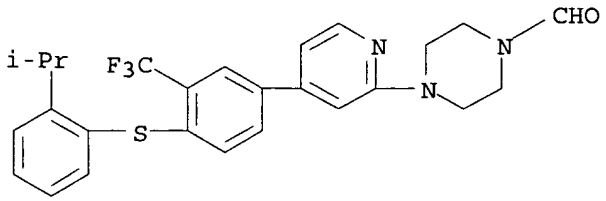
Absolute stereochemistry.



RN 388117-90-6 HCAPLUS
CN 4-Piperidinol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

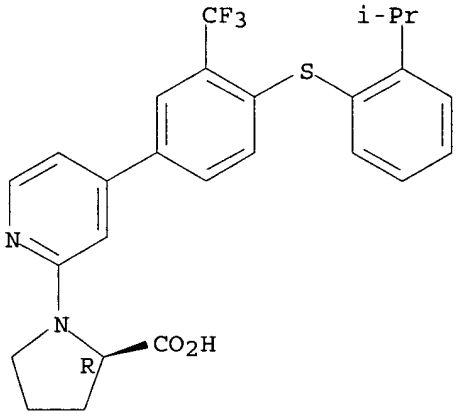


RN 388117-91-7 HCAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

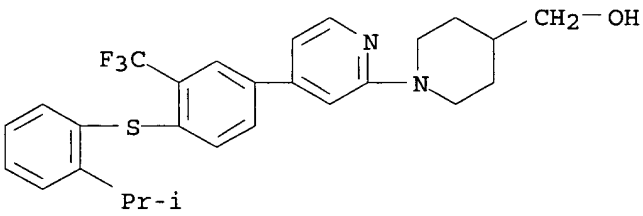


RN 388117-92-8 HCAPLUS
CN D-Proline, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

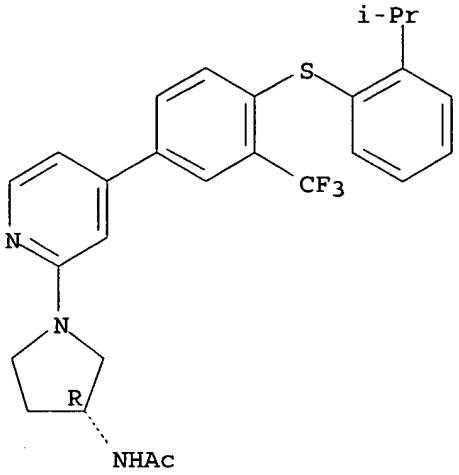


RN 388117-93-9 HCAPLUS
CN 4-Piperidinemethanol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

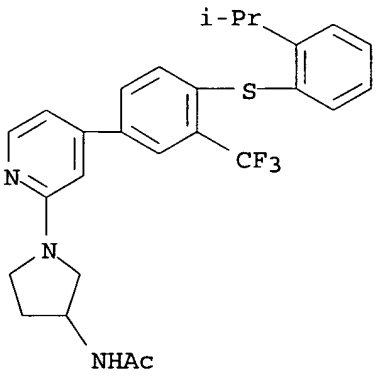


RN 388117-94-0 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

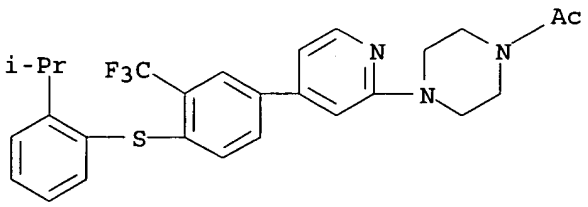
Absolute stereochemistry.



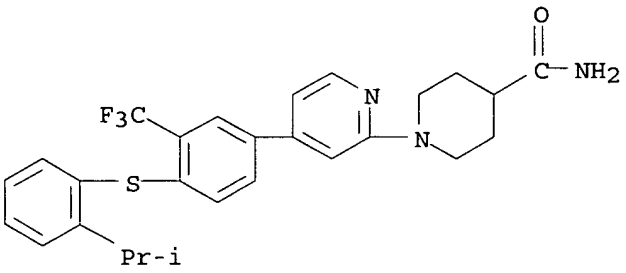
RN 388117-95-1 HCAPLUS
CN Acetamide, N-[1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)



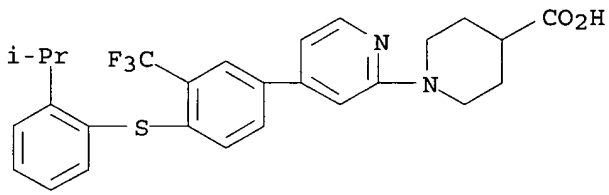
RN 388117-96-2 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



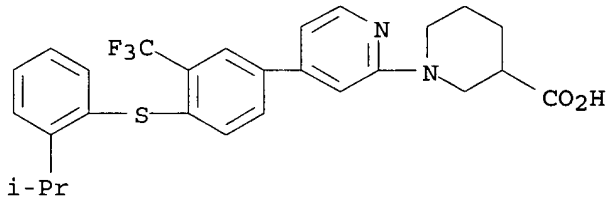
RN 388117-97-3 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



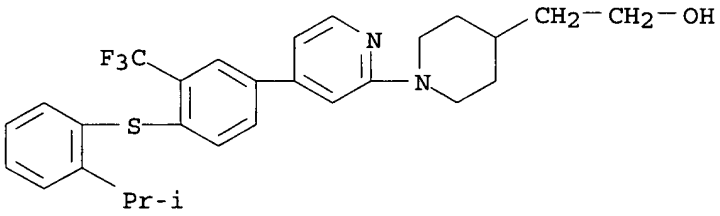
RN 388117-98-4 HCAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388117-99-5 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

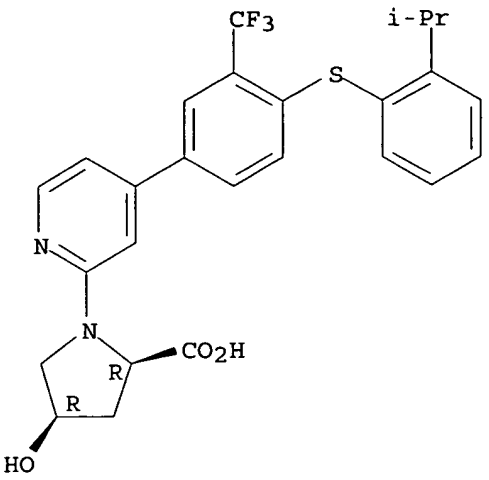


RN 388118-00-1 HCAPLUS
CN 4-Piperidineethanol, 1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



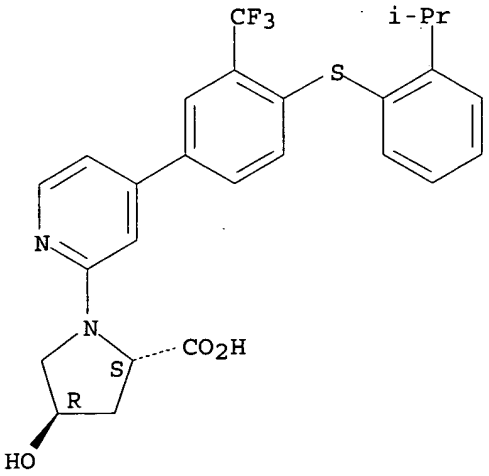
RN 388118-01-2 HCAPLUS
CN D-Proline, 4-hydroxy-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

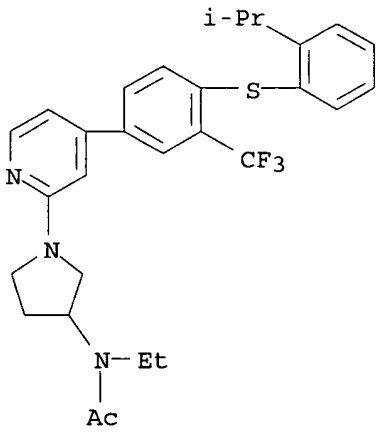


RN 388118-02-3 HCAPLUS
CN L-Proline, 4-hydroxy-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

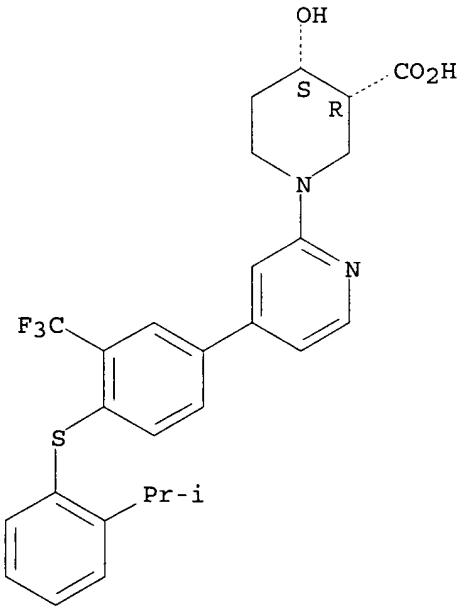


RN 388118-03-4 HCAPLUS
CN Acetamide, N-ethyl-N-[1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

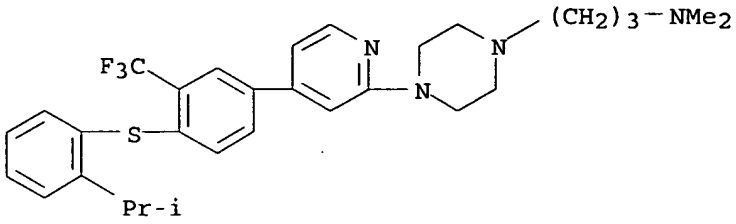


RN 388118-04-5 HCAPLUS
CN 3-Piperidinecarboxylic acid, 4-hydroxy-1-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

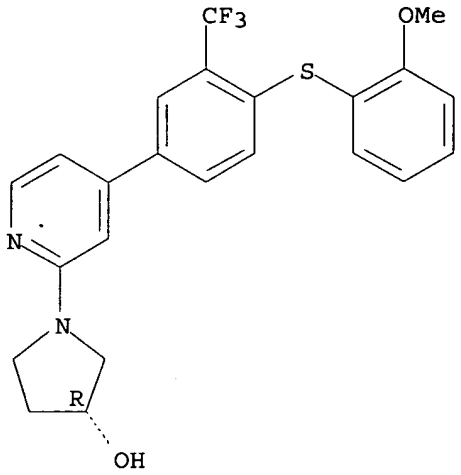


RN 388118-05-6 HCAPLUS
CN 1-Piperazinepropanamine, N,N-dimethyl-4-[4-[4-[[2-(1-methylethyl)phenyl]thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



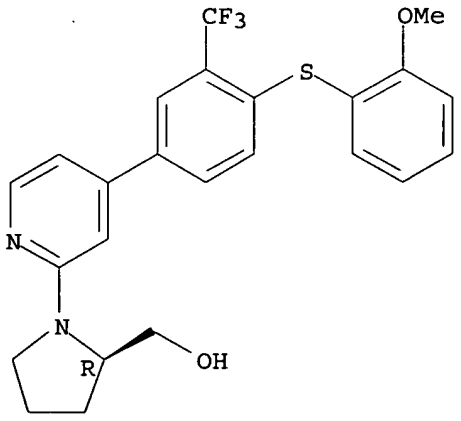
RN 388118-06-7 HCAPLUS
CN 3-Pyrrolidinol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



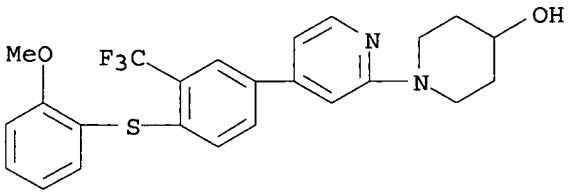
RN 388118-07-8 HCAPLUS
CN 2-Pyrrolidinemethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

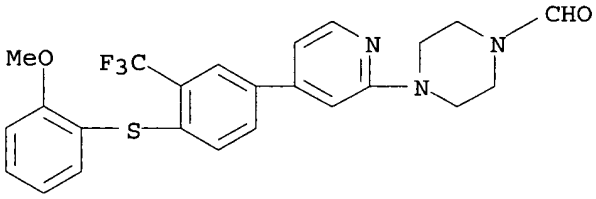


RN 388118-08-9 HCAPLUS

CN 4-Piperidinol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

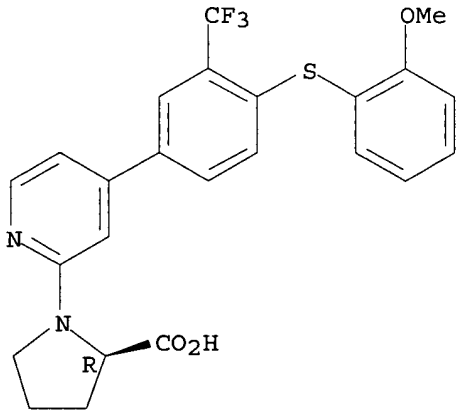


RN 388118-09-0 HCAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

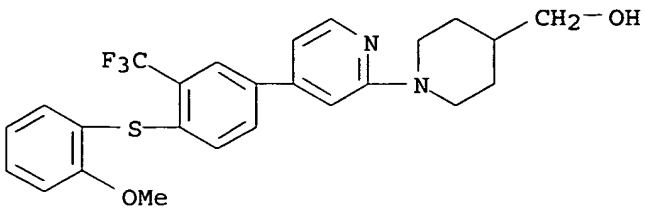


RN 388118-10-3 HCAPLUS
CN D-Proline, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

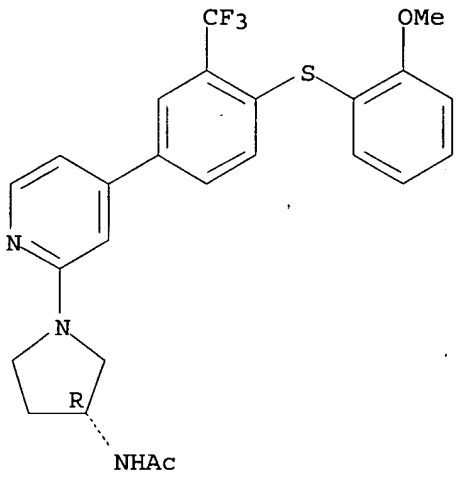


RN 388118-11-4 HCAPLUS
CN 4-Piperidinemethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

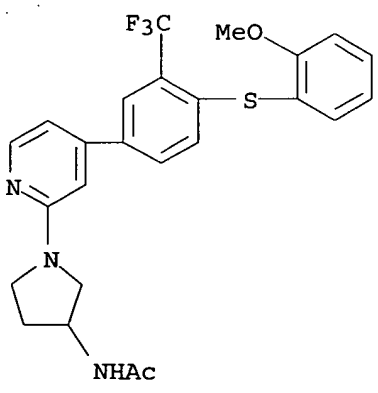


RN 388118-12-5 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

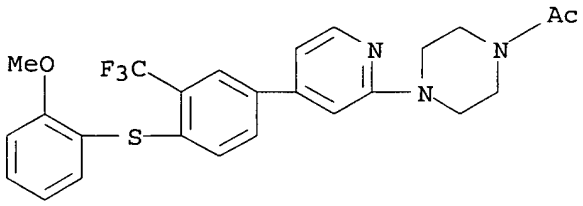
Absolute stereochemistry.



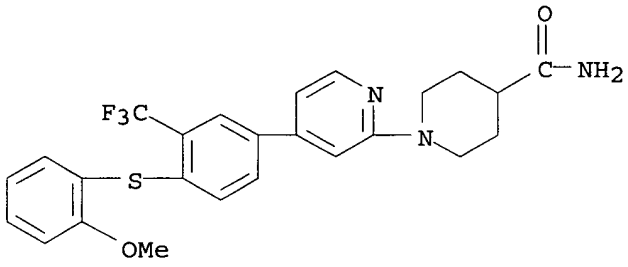
RN 388118-13-6 HCAPLUS
CN Acetamide, N-[1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)



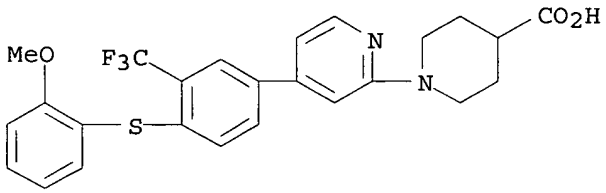
RN 388118-14-7 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



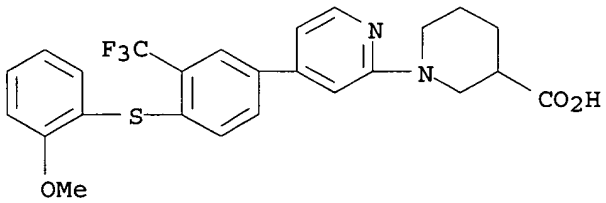
RN 388118-15-8 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



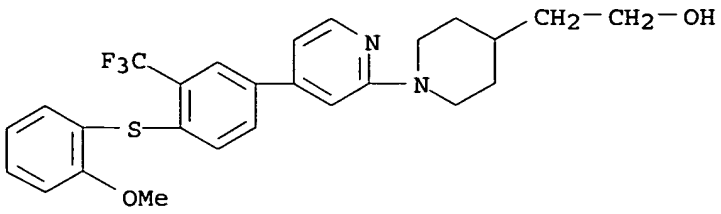
RN 388118-16-9 HCAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388118-17-0 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

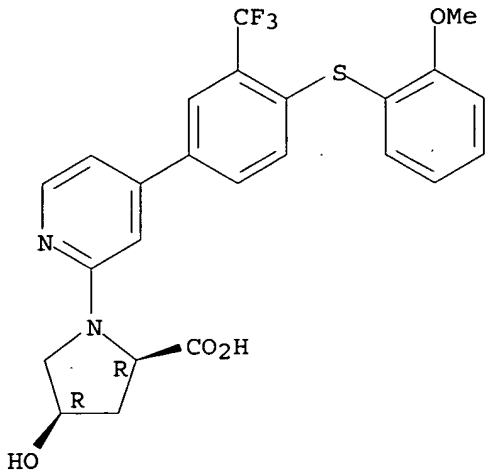


RN 388118-18-1 HCAPLUS
CN 4-Piperidineethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



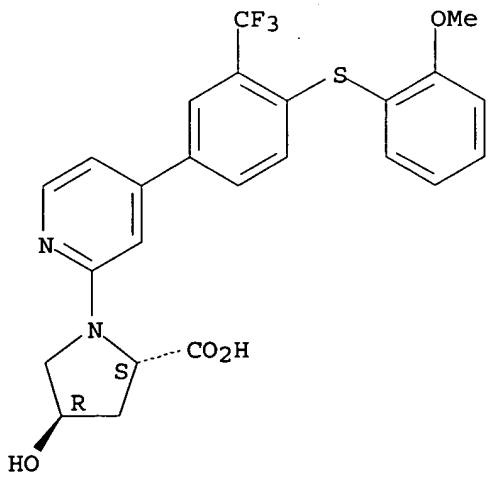
RN 388118-19-2 HCAPLUS
CN D-Proline, 4-hydroxy-1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

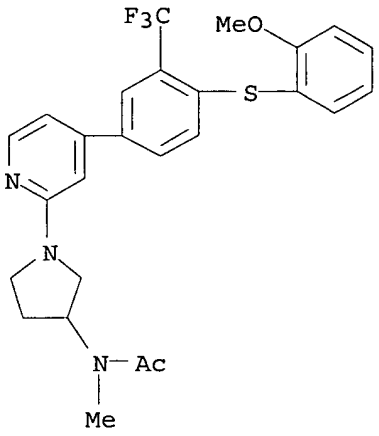


RN 388118-20-5 HCAPLUS
CN L-Proline, 4-hydroxy-1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (4R)- (9CI) (CA INDEX NAME)

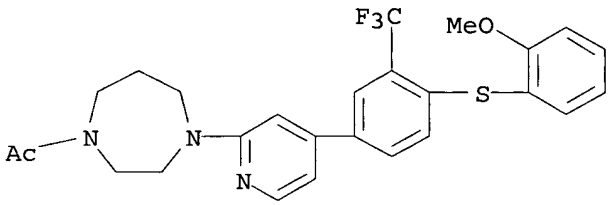
Absolute stereochemistry.



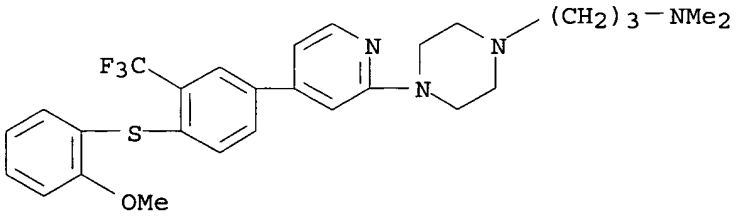
RN 388118-21-6 HCAPLUS
CN Acetamide, N-[1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]-N-methyl- (9CI) (CA INDEX NAME)



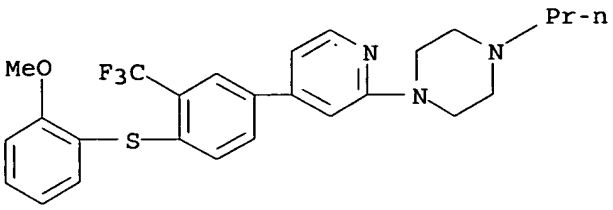
RN 388118-22-7 HCAPLUS
CN 1H-1,4-Diazepine, 1-acetylhexahydro-4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



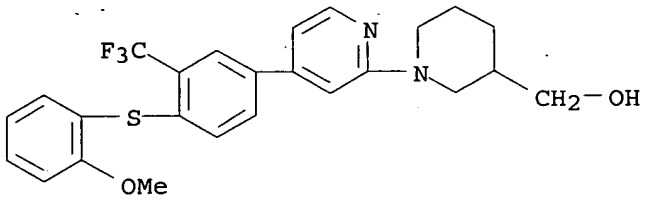
RN 388118-23-8 HCAPLUS
CN 1-Piperazinepropanamine, 4-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 388118-24-9 HCAPLUS
CN Piperazine, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-propyl- (9CI) (CA INDEX NAME)

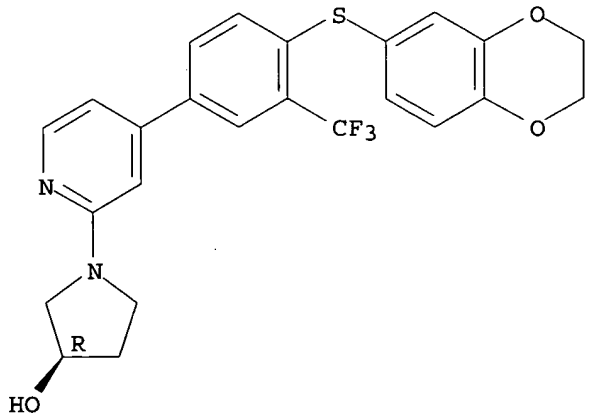


RN 388118-25-0 HCAPLUS
CN 3-Piperidinemethanol, 1-[4-[4-[(2-methoxyphenyl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

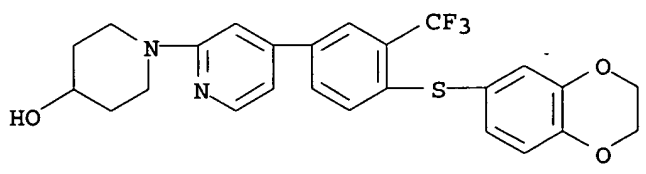


RN 388118-26-1 HCAPLUS
CN 3-Pyrrolidinol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

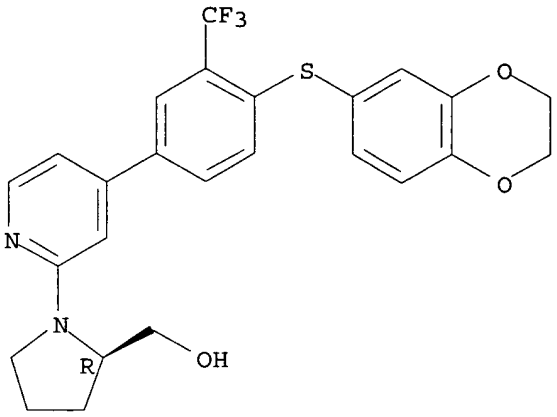


RN 388118-27-2 HCAPLUS
CN 4-Piperidinol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



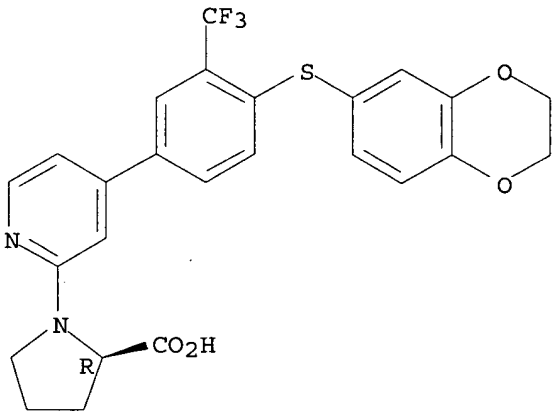
RN 388118-28-3 HCAPLUS
CN 2-Pyrrolidinemethanol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

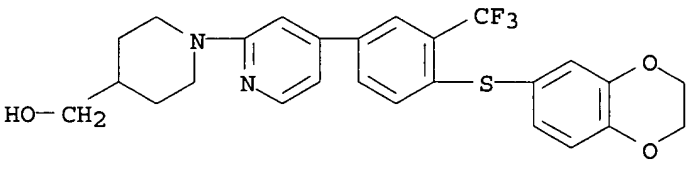


RN 388118-29-4 HCAPLUS
CN D-Proline, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

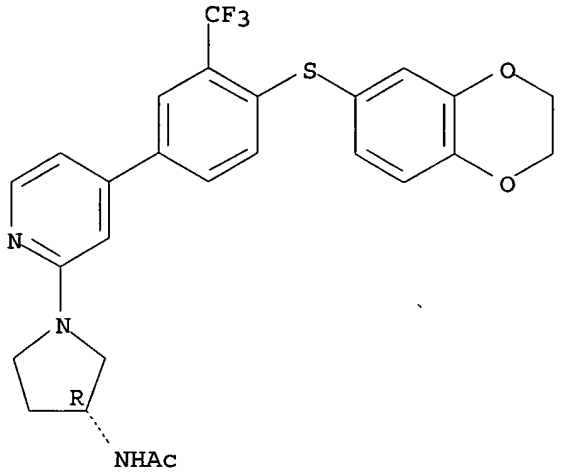


RN 388118-30-7 HCAPLUS
CN 4-Piperidinemethanol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

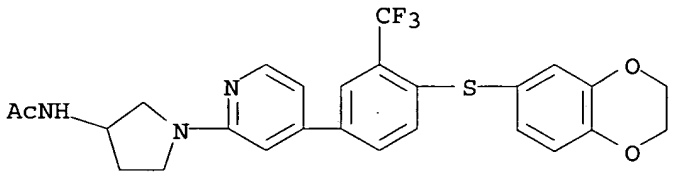


RN 388118-31-8 HCAPLUS
CN Acetamide, N-[(3R)-1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

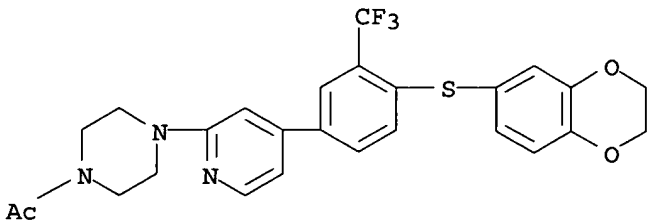
Absolute stereochemistry.



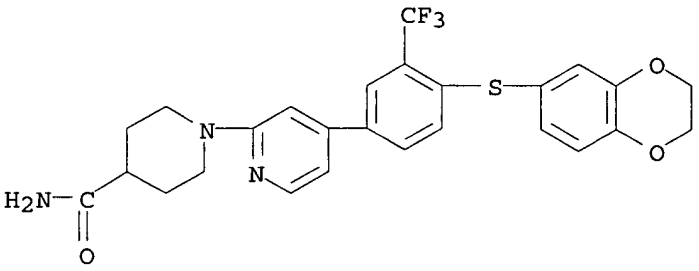
RN 388118-32-9 HCAPLUS
CN Acetamide, N-[1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)



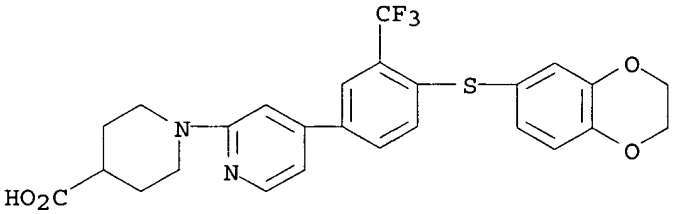
RN 388118-33-0 HCAPLUS
CN Piperazine, 1-acetyl-4-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



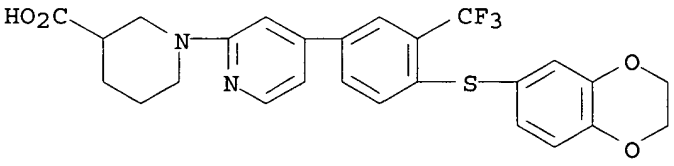
RN 388118-34-1 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



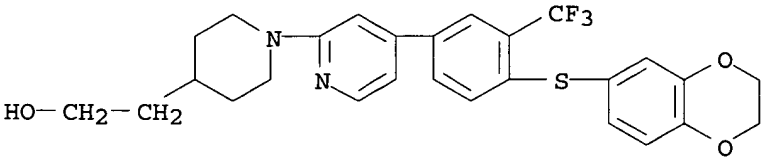
RN 388118-35-2 HCAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388118-36-3 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

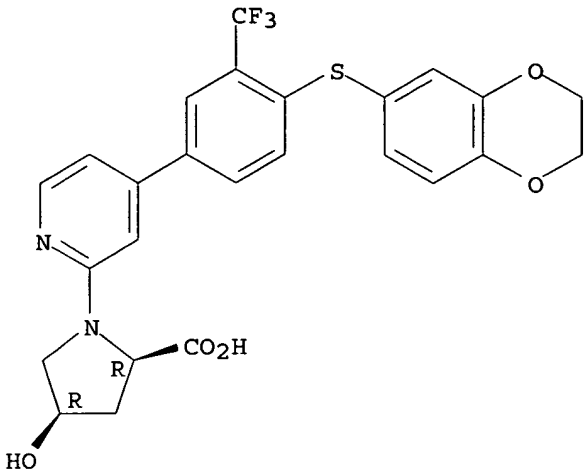


RN 388118-37-4 HCAPLUS
CN 4-Piperidineethanol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



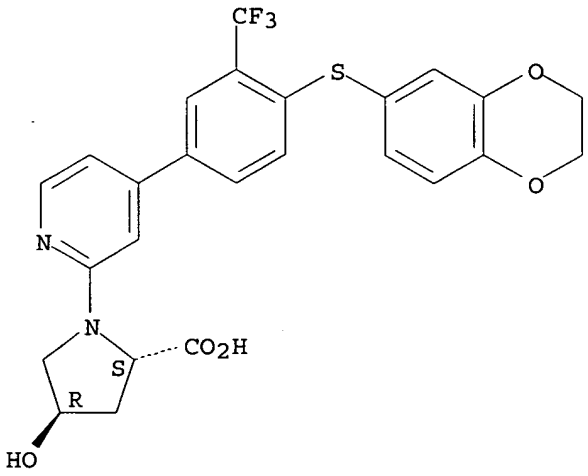
RN 388118-38-5 HCAPLUS
CN D-Proline, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-hydroxy-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

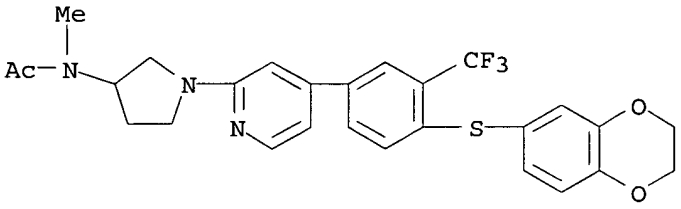


RN 388118-39-6 HCAPLUS
CN L-Proline, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-hydroxy-, (4R)- (9CI) (CA INDEX NAME)

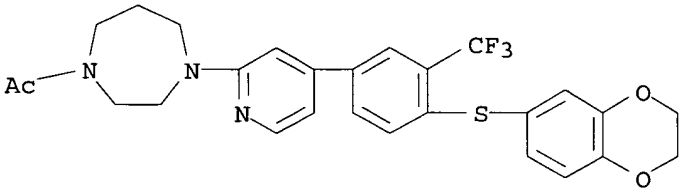
Absolute stereochemistry.



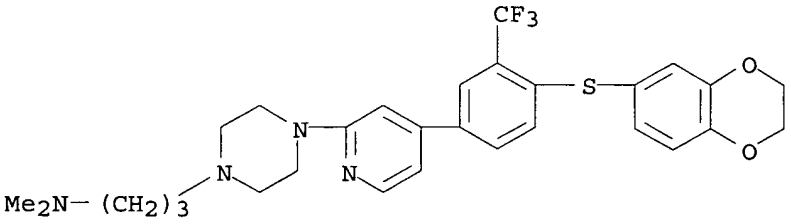
RN 388118-40-9 HCAPLUS
CN Acetamide, N-[1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-3-pyrrolidinyl]-N-methyl- (9CI) (CA INDEX NAME)



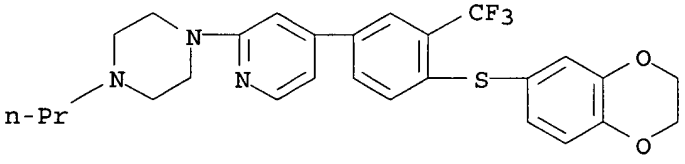
RN 388118-41-0 HCAPLUS
CN 1H-1,4-Diazepine, 1-acetyl-4-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]hexahydro- (9CI) (CA INDEX NAME)



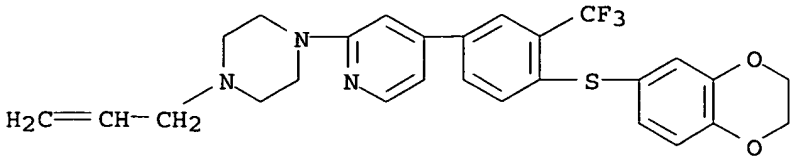
RN 388118-42-1 HCAPLUS
CN 1-Piperazinepropanamine, 4-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



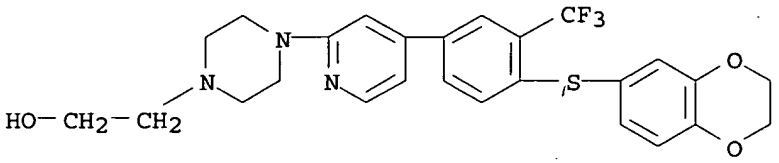
RN 388118-43-2 HCAPLUS
CN Piperazine, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-propyl- (9CI) (CA INDEX NAME)



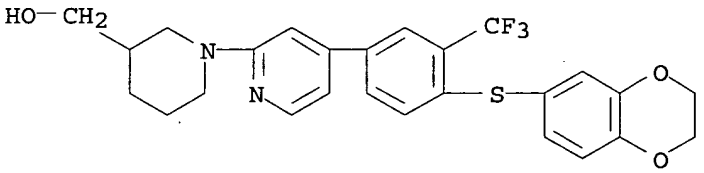
RN 388118-44-3 HCAPLUS
CN Piperazine, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]-4-(2-propenyl)- (9CI) (CA INDEX NAME)



RN 388118-45-4 HCAPLUS
CN 1-Piperazineethanol, 4-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 388118-46-5 HCAPLUS
CN 3-Piperidinemethanol, 1-[4-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

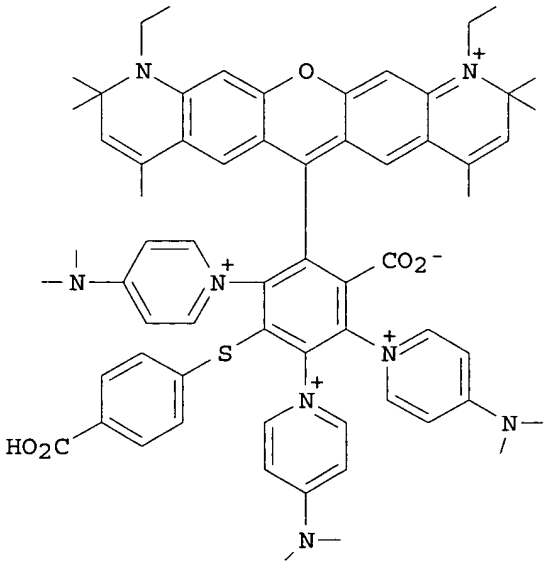
L12 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:338638 HCAPLUS
DOCUMENT NUMBER: 134:350265
TITLE: Water-soluble red-emitting fluorescent rhodamine dyes and energy-transfer dye pairs and conjugates for assays and stains
INVENTOR(S): Lee, Linda G.; Graham, Ronald J.; Werner, William E.; Swartzman, Elana; Lu, Lily
PATENT ASSIGNEE(S): PE Corporation, USA
SOURCE: PCT Int. Appl., 172 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032783	A1	20010510	WO 2000-US30414	20001101
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,				

LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU,
ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6191278	B1	20010220	US 1999-433093		19991103
US 6372907	B1	20020416	US 2000-661206		20000914
CA 2358923	AA	20010510	CA 2000-2358923		20001101
EP 1141137	A1	20011010	EP 2000-982085		20001101
EP 1141137	B1	20031008			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2003514058	T2	20030415	JP 2001-535469		20001101
AT 251658	E	20031015	AT 2000-982085		20001101
AU 770445	B2	20040219	AU 2001-19157		20001101
PRIORITY APPLN. INFO.:			US 1999-433093	A	19991103
			US 2000-661206	A	20000914
			WO 2000-US30414	W	20001101

OTHER SOURCE(S): MARPAT 134:350265
GI



I

AB The present invention provides novel, water-soluble, red-emitting fluorescent rhodamine dyes and red-emitting fluorescent energy-transfer dye pairs, as well as labeled conjugates comprising the same and methods for their use. The dyes, energy-transfer dye pairs and labeled conjugates are useful in a variety of aqueous-based applications, particularly in assays involving staining of cells, protein binding, and/or anal. of nucleic acids, such as hybridization assays and nucleic acid sequencing. A fluorescent-linked immunosorbent assay (FLISA) for human IL-8 used anti-human IL-8 antibody conjugated with rhodamine dye I (preparation given) and monoclonal anti-human IL-8 antibody-coated beads.

IT **339150-30-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(as rhodamine dye; water-soluble red-emitting fluorescent rhodamine dyes and energy-transfer dye pairs and conjugates for assays and stains)
RN 339150-30-0 HCAPLUS
CN Pyridinium, 1,1',1''-[6-carboxy-5-[1-[(4-carboxyphenyl)methyl]-11-ethyl-1,2,10,11-tetrahydro-2,2,4,8,10,10-hexamethylpyrano[3,2-g:5,6-g']diquinolin-13-ium-6-yl]-3-(phenylthio)-1,2,4-benzenetriyl]tris[4-(dimethylamino)-, mono(inner salt) (9CI) (CA INDEX NAME)

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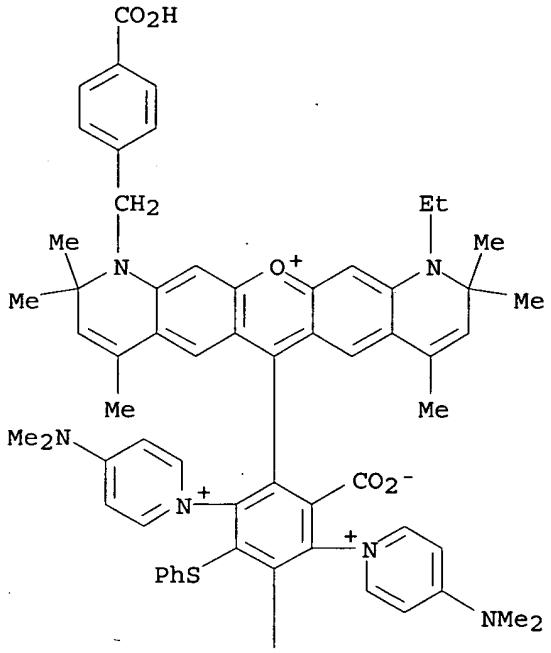
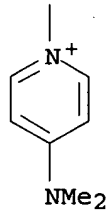


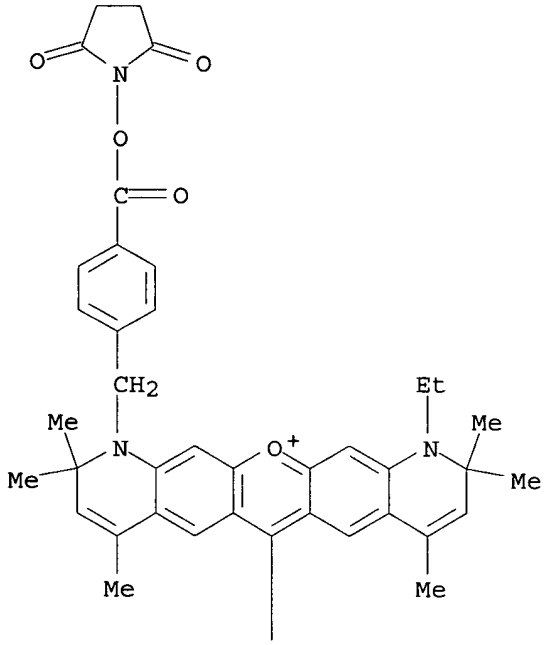
PAGE 2-A



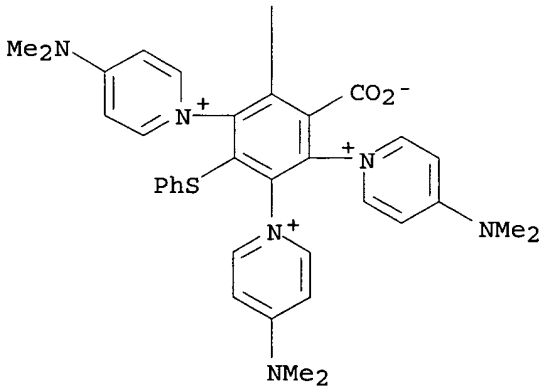
IT **339150-31-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(water-soluble red-emitting fluorescent rhodamine dyes and energy-transfer dye pairs and conjugates for assays and stains)
RN 339150-31-1 HCAPLUS
CN Pyridinium, 1,1',1''-[6-carboxy-5-[1-[[4-[[(2,5-dioxo-1-

pyrrolidinyl)oxy]carbonyl]phenyl]methyl]-11-ethyl-2,2,4,8,10,10-hexamethylpyrano[3,2-g:5,6-g']diquinolin-13-ium-6-yl]-3-(phenylthio)-1,2,4-benzenetriyl]tris[4-(dimethylamino)-, mono(inner salt) (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:131227 HCAPLUS
DOCUMENT NUMBER: 134:179914

TITLE: Water-soluble rhodamine dyes and conjugates thereof
INVENTOR(S): Lee, Linda G.; Graham, Ronald J.; Werner, William E.; Swartzman, Elana; Lu, Lily
PATENT ASSIGNEE(S): PE Corp., USA
SOURCE: U.S., 52 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6191278	B1	20010220	US 1999-433093	19991103
US 6372907	B1	20020416	US 2000-661206	20000914
CA 2358923	AA	20010510	CA 2000-2358923	20001101
WO 2001032783	A1	20010510	WO 2000-US30414	20001101
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1141137	A1	20011010	EP 2000-982085	20001101
EP 1141137	B1	20031008		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003514058	T2	20030415	JP 2001-535469	20001101
AT 251658	E	20031015	AT 2000-982085	20001101
AU 770445	B2	20040219	AU 2001-19157	20001101
ES 2206333	T3	20040516	ES 2000-982085	20001101
US 2003055257	A1	20030320	US 2001-7253	20011024

PRIORITY APPLN. INFO.:		
US 1999-433093	A3	19991103
US 2000-661206	A	20000914
WO 2000-US30414	W	20001101

OTHER SOURCE(S): MARPAT 134:179914

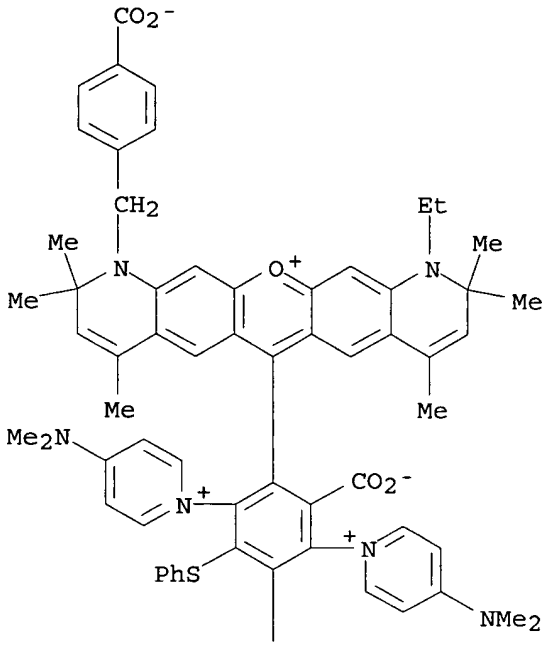
AB The present invention provides novel, water-soluble, red-emitting fluorescent rhodamine dyes and red-emitting fluorescent energy-transfer dye pairs, as well as labeled conjugates comprising the same and methods for their use. The dyes, energy-transfer dye pairs and labeled conjugates are useful in a variety of aqueous-based applications, particularly in assays involving staining of cells, protein binding, and/or anal. of nucleic acids, such as hybridization assays and nucleic acid sequencing.

IT **326801-79-0P**
RL: BUU (Biological use, unclassified); IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or engineered material use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(blue dye; production of fluorescent rhodamine dyes for biochem. labeling)

RN 326801-79-0 HCAPLUS

CN Pyridinium, 1,1',1''-[6-carboxy-5-[1-[(4-carboxyphenyl)methyl]-11-ethyl-1,2,10,11-tetrahydro-2,2,4,8,10,10-hexamethylpyrano[3,2-g:5,6-g']diquinolin-13-ium-6-yl]-3-(phenylthio)-1,2,4-benzenetriyl]tris[4-(dimethylamino)-, bis(inner salt) (9CI) (CA INDEX NAME)

PAGE 1-A



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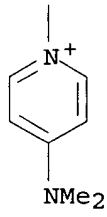
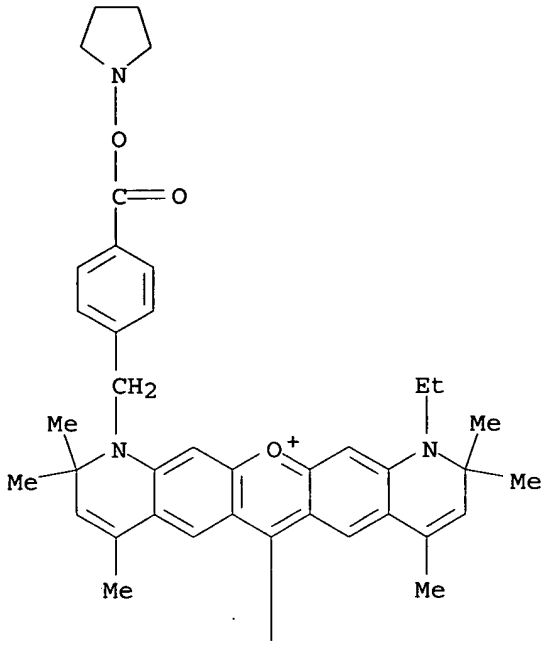
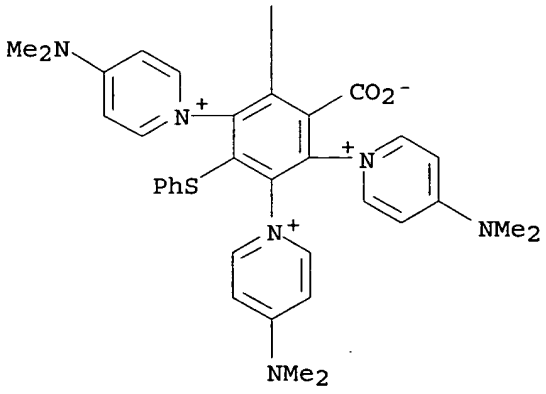


IT **326801-91-6P**
RL: BUU (Biological use, unclassified); IMF (Industrial manufacture); TEM (Technical or engineered material use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(blue dye; production of fluorescent rhodamine dyes for biochem. labeling)
RN 326801-91-6 HCAPLUS
CN Pyridinium, 1,1',1''-[6-carboxy-5-[1-ethyl-1,2,10,11-tetrahydro-2,2,4,8,10,10-hexamethyl-11-[[4-[(1-pyrrolidinyloxy)carbonyl]phenyl]methyl]pyrano[3,2-g:5,6-g']diquinolin-13-ium-6-yl]-3-(phenylthio)-1,2,4-benzenetriyl]tris[4-(dimethylamino)-, mono(inner salt) (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



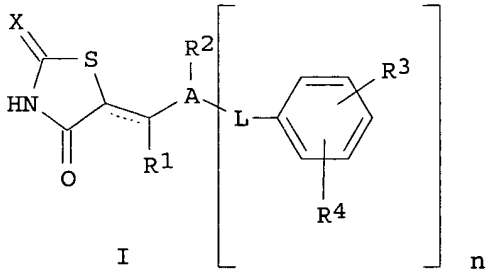
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:31481 HCAPLUS
DOCUMENT NUMBER: 134:100859
TITLE: Preparation of 2,4-dioxothiazolidines and 4-oxo-2-thioxothiazolidines having telomerase inhibitory activity and methods of their use
INVENTOR(S): Chin, Allison C.; Holcomb, Ryan; Piatyszek, Mieczyslaw A.; Singh, Upinder; Tolman, Richard L.; Akama, Tsutomu; Kanda, Yutaka; Asai, Akira; Yamashita,

Yoshinori; Endo, Kaori; Yamaguchi, Hiroyuki
PATENT ASSIGNEE(S): Geron Corporation, USA; Kyowa Hakko Kogyo Co., Ltd.
SOURCE: PCT Int. Appl., 211 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001002377	A1	20010111	WO 2000-US18211		20000630
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
JP 2001072592	A2	20010321	JP 1999-307576		19991028
CA 2341253	AA	20010111	CA 2000-2341253		20000630
EP 1109796	A1	20010627	EP 2000-950282		20000630
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
US 6518268	B1	20030211	US 2000-608636		20000630
JP 2003507473	T2	20030225	JP 2001-518671		20000630
US 2002115700	A1	20020822	US 2002-77738		20020213
PRIORITY APPLN. INFO.:			JP 1999-187616	A	19990701
			US 1999-142173P	P	19990701
			JP 1999-307576	A	19991028
			US 2000-608861	A1	20000630
			WO 2000-US18211	W	20000630

OTHER SOURCE(S): MARPAT 134:100859
GI



I

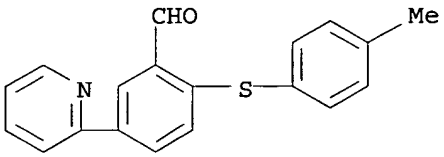
AB Thiazolidinedione compds. (shown as I; e.g. 5-((2-(4-chlorophenylthio)-5-nitrophenyl)methylene)-2,4-thiazolidinedione), compns., and methods of inhibiting telomerase activity in vitro and treatment of telomerase-mediated conditions or diseases ex vivo and in vivo are provided. In I, X = O or S; the dashed bond is a single or double bond; A = aryl or heteroaryl; R1 = H or lower alkyl; R2, R3 and R4 are independently selected from H, halo, alkyl, aryl, hydroxyl, alkoxyl, aryloxy, aralkoxy, cyano, nitro, alkylcarbamido, arylcarbamido,

dialkylcarbamido, diarylcarbamido, alkylarylcarbamido, alkylthiocarbamido, arylthiocarbamido, dialkylthiocarbamido, diarylthiocarbamido, alkylarylthiocarbamido, amino, alkylamino, arylamino, dialkylamino, diarylamino, arylalkylamino, aminocarbonyl, alkylaminocarbonyl, arylaminocarbonyl, dialkylaminocarbonyl, diarylaminocarbonyl, arylalkylaminocarbonyl, alkylcarbonyloxy, arylcarbonyloxy, carboxyl, alkoxycarbonyl, aryloxycarbonyl, sulfo, alkylsulfonylamido, arylsulfonylamido, alkylsulfonyl, arylsulfonyl, alkylsulfinyl, arylsulfinyl and heteroaryl; L is a direct bond or a linking group having from 1 to 3 unsubstituted or substituted C, N, O or S atoms; and n = 1, 2. A pharmaceutically acceptable salt thereof is also claimed. The methods, compds. and compns. of the invention may be employed alone, or in combination with other pharmacol. active agents in the treatment of conditions or diseases mediated by telomerase activity, such as in the treatment of cancer. Also disclosed are novel methods for assaying or screening for inhibitors of telomerase activity. More than 200 example prepns. are included, but the methods of preparation are not claimed.

IT **319454-78-9P**, 2-[(4-Methylphenyl)thio]-5-(2-pyridyl)benzaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; for preparation of 2,4-dioxothiazolidines and 4-oxo-2-thioxothiazolidines having telomerase inhibitory activity)

RN 319454-78-9 HCAPLUS

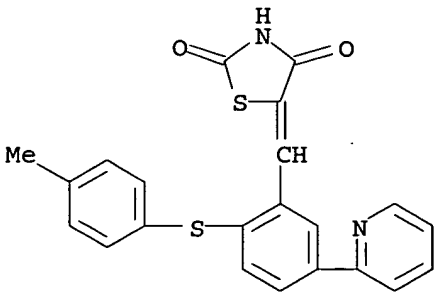
CN Benzaldehyde, 2-[(4-methylphenyl)thio]-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)



IT **319453-29-7P**, 5-((2-(4-Methylphenylthio)-5-(2-pyridinyl)phenyl)methylene)-2,4-thiazolidinedione
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2,4-dioxothiazolidines and 4-oxo-2-thioxothiazolidines having telomerase inhibitory activity and methods of use)

RN 319453-29-7 HCAPLUS

CN 2,4-Thiazolidinedione, 5-[[2-[(4-methylphenyl)thio]-5-(2-pyridinyl)phenyl]methylene]- (9CI) (CA INDEX NAME)



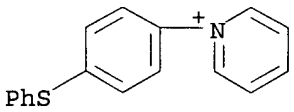
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:527570 HCAPLUS
DOCUMENT NUMBER: 131:249432
TITLE: Mono- and bimolecular reactions of electrogenerated diaryl sulfide radical cations and dications
AUTHOR(S): Zhuikov, V. V.
CORPORATE SOURCE: Kazan State University, Kazan, Russia
SOURCE: Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii) (1999), 69(3), 502-503
CODEN: RJGCEK; ISSN: 1070-3632
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English

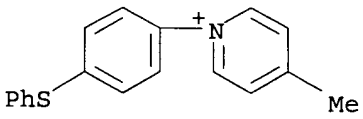
AB The electrochem. oxidation of diaryl sulfides was carried out in MeCN/0.01M Et4NBF4 on Pt oxide rotating disk electrode. By the switching technique formation of short-lived radical cations was detected. The electrochem. oxidation of diaryl sulfides ((p-RC6H4)2S, R = H, MeO, Me, Cl) on the Pt oxide rotating disk electrode has two waves and the shape of the wave and the other dependencies suggest that the chemical reaction of the radical cations is second order. Oxidation of Ph2S in the presence of pyridine leads to formation of N-(p-phenylthiophenyl)pyridinium salts with the yields considerably lower going from pyridine to γ-picoline to α-picoline to 2,6-lutidine, which evidently arise from different basicities and nucleophilicities of the pyridine derivs. Intramol. electronic interactions and the nature of approaching foreign nucleophilic reagent can affect the mechanism of reaction of the intermediates.

IT **92639-74-2DP**, salts **117186-17-1DP**, salts **244215-09-6DP**, salts **244215-11-0DP**, salts
RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(preparation in electrochem. oxidation of di-Ph disulfide in presence of pyridine)

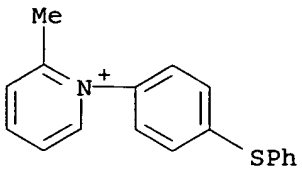
RN 92639-74-2 HCAPLUS
CN Pyridinium, 1-[4-(phenylthio)phenyl]- (9CI) (CA INDEX NAME)



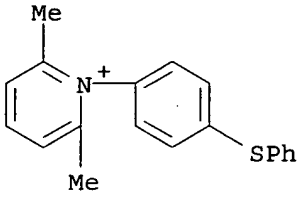
RN 117186-17-1 HCAPLUS
CN Pyridinium, 4-methyl-1-[4-(phenylthio)phenyl]- (9CI) (CA INDEX NAME)



RN 244215-09-6 HCAPLUS
CN Pyridinium, 2-methyl-1-[4-(phenylthio)phenyl]- (9CI) (CA INDEX NAME)



RN 244215-11-0 HCAPLUS
CN Pyridinium, 2,6-dimethyl-1-[4-(phenylthio)phenyl]- (9CI) (CA INDEX NAME)



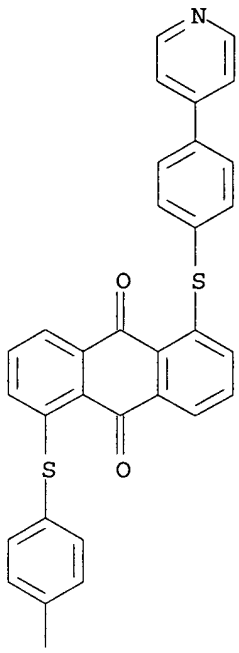
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:779499 HCAPLUS
DOCUMENT NUMBER: 130:88236
TITLE: Guest-host type liquid crystal display with improved brightness
INVENTOR(S): Iwanaga, Hironori; Naito, Katsuyuki
PATENT ASSIGNEE(S): Toshiba Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 10316970	A2	19981202	JP 1997-71587		19970325
US 6057906	A	20000502	US 1997-825179		19970327
KR 228465	B1	19991101	KR 1997-11507		19970329
PRIORITY APPLN. INFO.:			JP 1996-75614	A	19960329
			JP 1996-236780	A	19960906
			JP 1997-65145	A	19970318

OTHER SOURCE(S): MARPAT 130:88236
AB The title display utilizes at least 1 dichroic dye containing thiocarbonyl, thioester, dithioester, selenocarbonyl, selenoester and/or diselenoester. The liquid crystal composition may contain a proton donor and a proton acceptor.
IT **218154-82-6**
RL: MOA (Modifier or additive use); USES (Uses)
(proton acceptor in liquid crystal composition for guest-host type liquid crystal display)
RN 218154-82-6 HCAPLUS
CN 9,10-Anthracenedione, 1-[(4-ethylphenyl)thio]-5-[[4-(4-pyridinyl)phenyl]thio]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

L12 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:621902 HCAPLUS
DOCUMENT NUMBER: 117:221902
TITLE: Electrochemical reactions of heteroorganic compounds
AUTHOR(S): Kargin, Yu. M.; Zhuikov, V. V.; Budnikova, Yu. G.; Fattakhova, D. S.
CORPORATE SOURCE: Kazan. Gos. Univ., Kazan, Russia
SOURCE: Elektrokhimiya (1992), 28(4), 615-28
CODEN: ELKKAX; ISSN: 0424-8570
DOCUMENT TYPE: Journal
LANGUAGE: Russian

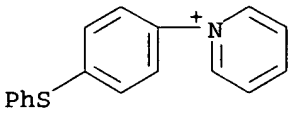
AB Processes are described of intermediates of heteroorg. compds. during fragmentation of ion radicals (with bond cleavage) and disproportionation and dimerization of cation radicals. Special attention is paid to reaction of Si- and P-containing compds. The electrochem. is described. Cation radicals with lower electron d. were characterized by the 2nd order reactions.

IT **92639-75-3P 92639-76-4P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. reaction of di-Ph sulfide in presence of organic additives)
RN 92639-75-3 HCAPLUS

CN Pyridinium, 1-[4-(phenylthio)phenyl]-, perchlorate (9CI) (CA INDEX NAME)

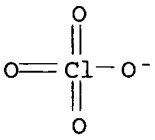
CM 1

CRN 92639-74-2
CMF C17 H14 N S



CM 2

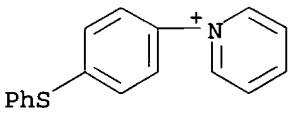
CRN 14797-73-0
CMF Cl O4



RN 92639-76-4 HCAPLUS
CN Pyridinium, 1-[4-(phenylthio)phenyl]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

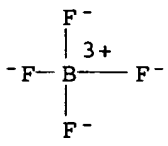
CM 1

CRN 92639-74-2
CMF C17 H14 N S



CM 2

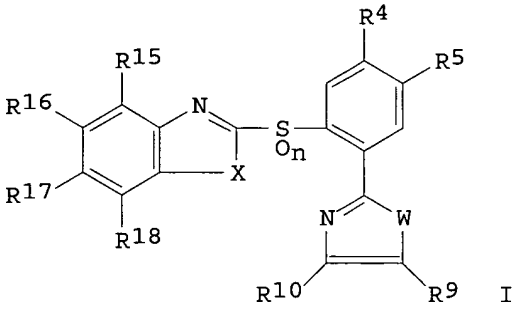
CRN 14874-70-5
CMF B F4
CCI CCS



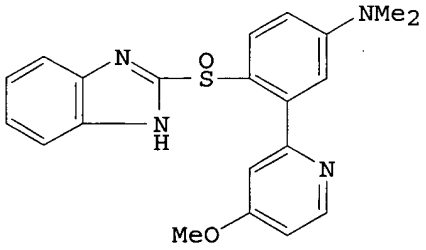
L12 ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:559137 HCAPLUS
DOCUMENT NUMBER: 115:159137
TITLE: Preparation of 2-(heteroarylphenylthio)benzimidazoles and related compounds as antiinflammatories and gastric acid secretion inhibitors
PATENT ASSIGNEE(S): Fisons PLC, UK
SOURCE: Austrian, 21 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 392788	B	19910610	AT 1988-223	19880203
AT 8800223	A	19901115		
PRIORITY APPLN. INFO.:			AT 1988-223	19880203

OTHER SOURCE(S): MARPAT 115:159137
GI



I

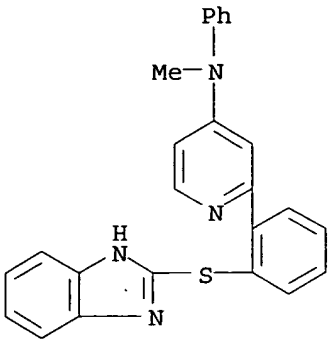


II

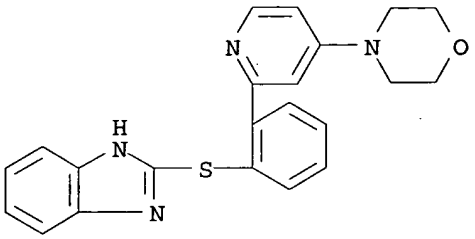
AB Title compds. [I; X = O, NR19; W = NR8, CR7:CR8; R4,R5 = H, alkyl, alkoxy, halo, amino; R7,R8 = H, alkyl, alkoxy, amino, morpholino, (substituted) alkoxy; R9,R10 = H, alkyl; R9R10 = atoms to complete a (halo-substituted) Ph ring; R15-R18 = H, alkyl, halo, alkoxy, NO2, amino, (modified) CO2H; R19 = H, (substituted) alkyl; n = 0,1], were prepared as antiinflammatories and gastric acid secretion inhibitors (no data). Thus, title compound II was prepared starting from 4-O2NC6H4N2BF4 and 4-methoxypyridine N-oxide and proceeding via 2-(2-mercapto-5-nitrophenyl)-4-methoxypyridine N,N-dimethylcarbonate.

IT **115741-52-1P 115741-80-5P 115741-82-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)

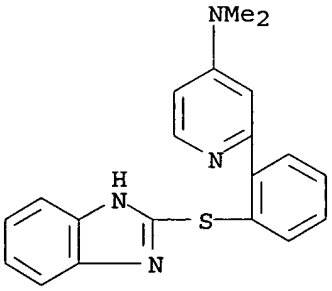
(preparation of, as antiinflammatory and gastric acid secretion inhibitor)
RN 115741-52-1 HCAPLUS
CN 4-Pyridinamine, 2-[2-(1H-benzimidazol-2-ylthio)phenyl]-N-methyl-N-phenyl- (9CI) (CA INDEX NAME)



RN 115741-80-5 HCAPLUS
CN 1H-Benzimidazole, 2-[[2-[4-(4-morpholinyl)-2-pyridinyl]phenyl]thio]- (9CI) (CA INDEX NAME)



RN 115741-82-7 HCAPLUS
CN 4-Pyridinamine, 2-[2-(1H-benzimidazol-2-ylthio)phenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

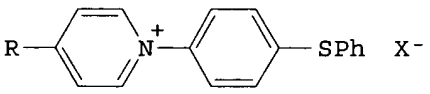


L12 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:590253 HCAPLUS
DOCUMENT NUMBER: 109:190253
TITLE: Preparation of N-[p-phenylthio)phenyl]pyridinium or -picolinium salts
INVENTOR(S): Latypova, V. Z.; Zhuikov, V. V.; Kargin, Yu. M.

PATENT ASSIGNEE(S): Kazan State University, USSR
SOURCE: U.S.S.R. From: Otkrytiya, Izobret. 1987, (42), 81.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 1351926	A1	19871115	SU 1986-4029681	19860224
PRIORITY APPLN. INFO.:			SU 1986-4029681	19860224

GI



I

AB Title compds. (I) (R = H, Me; X = ClO4, BF4) are prepared by electrochem. oxidation of Ph2S on a Pt electrode in MeCN in the presence of NaClO4 or Et4N+ BF4- and pyridine or γ-picoline at a 5-15 mA/cm2 c.d., at 15-25°, and change in the electrolysis potential from 1.1 to 2.2 V with subsequent evaporation of a solvent, washing the residue with a HClO4 solution, and extracting I with CHCl3.

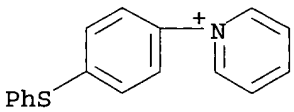
IT **92639-75-3P 92639-76-4P 117186-18-2P**
117186-19-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 92639-75-3 HCAPLUS

CN Pyridinium, 1-[4-(phenylthio)phenyl]-, perchlorate (9CI) (CA INDEX NAME)

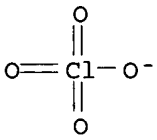
CM 1

CRN 92639-74-2
CMF C17 H14 N S



CM 2

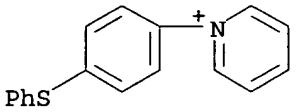
CRN 14797-73-0
CMF Cl O4



RN 92639-76-4 HCAPLUS
CN Pyridinium, 1-[4-(phenylthio)phenyl]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

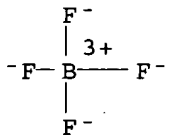
CM 1

CRN 92639-74-2
CMF C17 H14 N S



CM 2

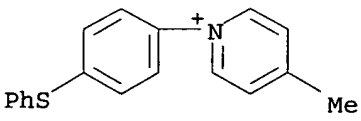
CRN 14874-70-5
CMF B F4
CCI CCS



RN 117186-18-2 HCAPLUS
CN Pyridinium, 4-methyl-1-[4-(phenylthio)phenyl]-, perchlorate (9CI) (CA INDEX NAME)

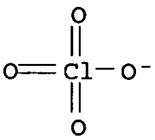
CM 1

CRN 117186-17-1
CMF C18 H16 N S



CM 2

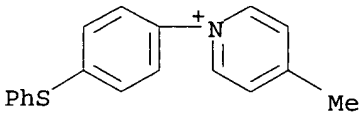
CRN 14797-73-0
CMF Cl O4



RN 117186-19-3 HCAPLUS
CN Pyridinium, 4-methyl-1-[4-(phenylthio)phenyl]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

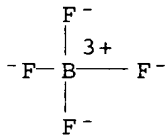
CM 1

CRN 117186-17-1
CMF C18 H16 N S



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



L12 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:493009 HCAPLUS
DOCUMENT NUMBER: 109:93009
TITLE: Preparation of heterocyclic-substituted azoles as gastric secretion inhibitors and antiinflammatories
INVENTOR(S): Cox, David; Dowlatshahi, Hossein Ali; Hall, David Edward Hall; Ingall, Anthony Howard; Suschitzky, John Louis
PATENT ASSIGNEE(S): Fisons PLC, UK
SOURCE: Eur. Pat. Appl., 36 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 262845	A1	19880406	EP 1987-308318	19870921
R: ES, GR				
WO 8802367	A1	19880407	WO 1987-GB656	19870921
W: AU, DK, FI, JP, KR, NO				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8780244	A1	19880421	AU 1987-80244	19870921
AU 604771	B2	19910103		
EP 283504	A1	19880928	EP 1987-906433	19870921

R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE

JP 01501473	T2	19890525	JP 1987-505851		19870921
ZA 8707206	A	19880727	ZA 1987-7206		19870924
US 4900751	A	19900213	US 1987-100584		19870924
FI 8802394	A	19880520	FI 1988-2394		19880520
DK 8802876	A	19880701	DK 1988-2876		19880525
NO 8802321	A	19880711	NO 1988-2321		19880526
PRIORITY APPLN. INFO.:			GB 1986-23299	A	19860927
			GB 1986-23301	A	19860927
			GB 1987-5017	A	19870304
			GB 1987-19644	A	19870820
			US 1986-918832	A2	19861014
			WO 1987-GB656	A	19870921

OTHER SOURCE(S): MARPAT 109:93009

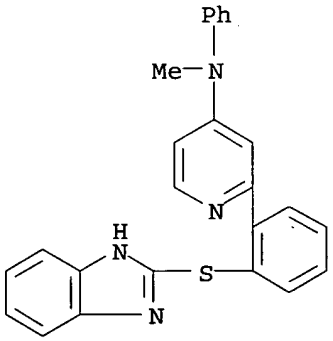
GI For diagram(s), see printed CA Issue.

AB The title compds. [I; R1, R2 = H, alkyl; R1R2 = atoms to complete an (un)substituted, fused benzo or pyrido ring; R3-R10 = H, alkyl, PhCO, amino (un)modified CO2H, (un)substituted alkoxy, heterocyclyl, etc.; X = O, S, R12N; R12 = H, (un)substituted alkyl; A = 5- or 6-membered, fully unsatd. carbocycle or heterocycle; B = 5- or 6-membered, fully unsatd., N-containing heterocycle; n = 0,1] and their pharmaceutically acceptable salts were prepared as gastric secretion and inflammation inhibitors (no data). 4-O2NC6H4N2+ BF4- was treated with 4-methoxypyridine 1-oxide to give 2-(4-methoxy-2-pyridinyl)-4-nitrophenol, which was esterified with Me2NCSCl and converted in 4 steps to give 4-(dimethylamino)-2-(4-methoxy-2-pyridinyl)phenyl disulfide. The latter was refluxed with 2-chlorobenzimidazole and NaBH3CN in HOAc/Me2CHOH to give (phenylthio)benzimidazole II.

IT **115741-52-1P 115741-80-5P 115741-82-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiinflammatory and gastric secretion inhibitor)

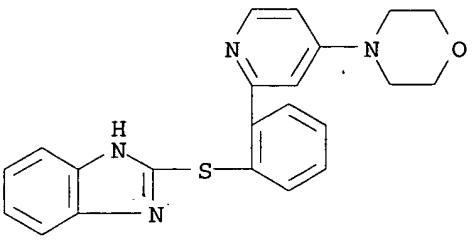
RN 115741-52-1 HCAPLUS

CN 4-Pyridinamine, 2-[2-(1H-benzimidazol-2-ylthio)phenyl]-N-methyl-N-phenyl- (9CI) (CA INDEX NAME)

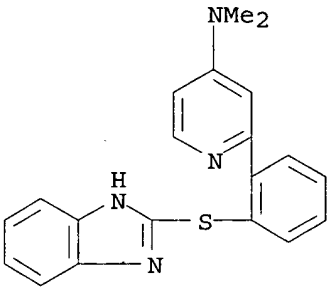


RN 115741-80-5 HCAPLUS

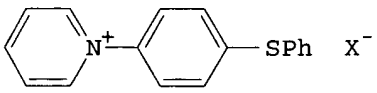
CN 1H-Benzimidazole, 2-[[2-[4-(4-morpholinyl)-2-pyridinyl]phenyl]thio]- (9CI) (CA INDEX NAME)



RN 115741-82-7 HCAPLUS
CN 4-Pyridinamine, 2-[2-(1H-benzimidazol-2-ylthio)phenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



L12 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:590876 HCAPLUS
DOCUMENT NUMBER: 101:190876
TITLE: Electrochemical reactions of sulfur-, selenium-, and tellurium-containing organic compounds. XIII. Oxidation of diphenyl sulfide
AUTHOR(S): Latypova, V. Z.; Yakovleva, O. G.; Zhuikov, V. V.; Khusaenov, N. M.; Chichirov, A. A.; Kargin, Yu. M.; Il'yasov, A. V.; Ismaev, I. E.
CORPORATE SOURCE: Kazan. Univ., Kazan, USSR
SOURCE: Zhurnal Obshchei Khimii (1984), 54(5), 1085-9
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



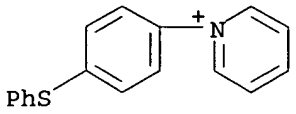
I

AB The electrochem. oxidation of Ph2S in MeCN-NaClO4 produced the cation radical, which disproportionated to form the dication; the latter reacted with certain nucleophiles. When pyridine was present, pyridinium salts I (X = ClO4, BF4) could be obtained.
IT **92639-75-3P 92639-76-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 92639-75-3 HCAPLUS

CN Pyridinium, 1-[4-(phenylthio)phenyl]-, perchlorate (9CI) (CA INDEX NAME)

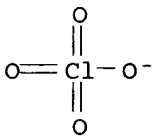
CM 1

CRN 92639-74-2
CMF C17 H14 N S



CM 2

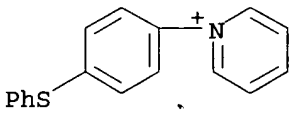
CRN 14797-73-0
CMF Cl O4



RN 92639-76-4 HCAPLUS
CN Pyridinium, 1-[4-(phenylthio)phenyl]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

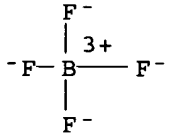
CM 1

CRN 92639-74-2
CMF C17 H14 N S



CM 2

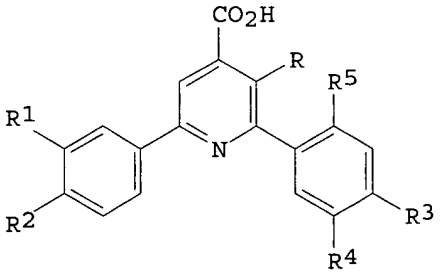
CRN 14874-70-5
CMF B F4
CCI CCS



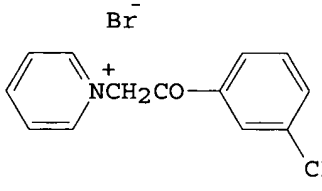
L12 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:125895 HCAPLUS
DOCUMENT NUMBER: 98:125895
TITLE: 2,6-Diarylpyridinecarboxylic acids and their therapeutic utility
INVENTOR(S): Skaletzsky, Louis Leonard
PATENT ASSIGNEE(S): Upjohn Co. , USA
SOURCE: Eur. Pat. Appl., 28 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 64385	A1	19821110	EP 1982-302180	19820428
EP 64385	B1	19860402		
R: BE, CH, DE, FR, GB, IT, NL, SE				
US 4377586	A	19830322	US 1981-259135	19810430
CA 1182397	A1	19850212	CA 1982-398962	19820322
ZA 8202249	A	19830223	ZA 1982-2249	19820401
JP 57185263	A2	19821115	JP 1982-70550	19820428
US 4474791	A	19841002	US 1982-449101	19821213
CA 1179676	A2	19841218	CA 1984-446371	19840130
PRIORITY APPLN. INFO.:			US 1981-259135 A	19810430
			CA 1982-398962 A3	19820322

GI



I

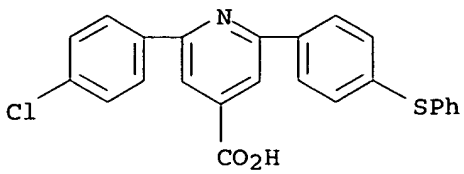


II

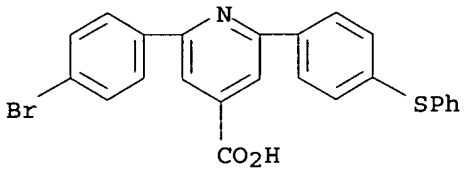
AB Antihypertensive (no data) diarylpyridinecarboxylates I [R = H, Me; R1 = H, F3C; R2 = H, Cl, F, Br, iodo, Me, CF3; R3 = H, Me, halo, F3C, Ph, PhO, 4-FC6H4, 4-FC6H4O; R4 = H, Cl, F, F3C, Me; R3R4 = (CH2)4, benzo; R5 = H, alkoxy, acetoxy] and their salts were prepared Thus, cyclocondensation of 4-BrC6H4COCH:CHCO2H, the pyridinium salt II and NH4OAc in refluxing MeOH containing HOAc gave 40% I (R = R1 = R3 = R5 = H; R2 = Br; R4 = F3C).

IT **85019-10-9P 85031-37-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

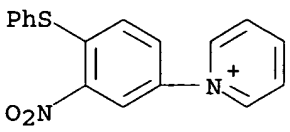
RN 85019-10-9 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2-(4-chlorophenyl)-6-[4-(phenylthio)phenyl]- (9CI) (CA INDEX NAME)



RN 85031-37-4 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2-(4-bromophenyl)-6-[4-(phenylthio)phenyl]-(9CI) (CA INDEX NAME)

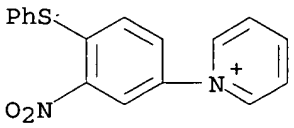


L12 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:448149 HCAPLUS
DOCUMENT NUMBER: 77:48149
TITLE: N-Phenylpyridinium salts. 2. Reactivity of N-(3-nitro-4-chlorophenyl)pyridinium chloride
AUTHOR(S): Lipke, Bodo; Lachmann, Christel; Schmidt, Reinhard
CORPORATE SOURCE: Sekt. Chem., Humboldt-Univ. Berlin, Berlin, Ger. Dem. Rep.
SOURCE: Zeitschrift fuer Chemie (1972), 12(3), 103-4
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The title compound (I) reacted with N2H4.H2O in boiling EtOH to give the hydrazino compound II only in small yields and as the benzylidene derivative III. III was obtained in increased yields by reaction of I with PhCH:NNH2. I and PhNHNH2 gave the triazolyl derivative IV. I and H2NNHCSNH2 or PhSH gave the corresponding thio ethers, which were cleaved with pyrrolidine to give 3,4-O2N(PhS)C6H3NH2 and 3,4-O2N(2-HO2CC6H4S)C6-H3NH2, resp. Similar cleavage of IV gave the expected 5-amino derivative V.
IT **37059-28-2P 37059-29-3P 37059-30-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 37059-28-2 HCAPLUS
CN Pyridinium, 1-[3-nitro-4-(phenylthio)phenyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

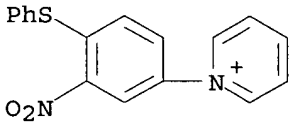
RN 37059-29-3 HCAPLUS
CN Pyridinium, 1-[3-nitro-4-(phenylthio)phenyl]-, iodide (9CI) (CA INDEX NAME)



RN 37059-30-6 HCAPLUS
CN Pyridinium, 1-[3-nitro-4-(phenylthio)phenyl]-, nitrate (9CI) (CA INDEX NAME)

CM 1

CRN 47226-33-5
CMF C17 H13 N2 O2 S



CM 2

CRN 14797-55-8
CMF N O3